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(71) Applicant (for all designated States except US): THE BOARD OF TRUSTEES OF THE LELAND STANFORD JUNIOR UNIVERSITY [US/US]; 1705 El Camino Real, Palo Alto, CA 94306-1106 (US).

(71) Applicants and

- (72) Inventors: SOLLID, Ludvig, M. [NO/NO]; Institute of Immunology, University of Oslo, Rikshospitalet, N-0027 Oslo (NO). HAUSCH, Felix [DE/CH]; Bergstrasse 57/205, CH-8032 Zurich (CH). SHAN, Lu [CN/US]; 63 Abrahms Ct. 4B, Stanford, CA 94305 (US). KHOSLA, Chaitan [US/US]; 740 La Para Avenue, Palo Alto, CA 94306 (US). QUARSTEN, Hanne [NO/NO]; Institute of Immunology, University of Oslo, Rikshospitalet, N-0027 Oslo (NO).
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): GRAY, Gary

[US/US]; 460 Gerona Road, Stanford, CA 94305 (US). **KIM, Chu-Young** [KR/US]; 4173 El Camino Real, No. 32, Palo Alto, CA 94306 (US).

- (74) Agent: SHERWOOD, Pamela, J.; Bozicevic, Field & Francis LLP, Suite 200, 200 Middlefield Road, Menlo Park, CA 94025 (US).
- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) Abstract: Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.





DRUG THERAPY FOR CELIAC SPRUE

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

BACKGROUND OF THE INVENTION

In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

[DQ(a1*03, b1*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a glutenfree diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

SUMMARY OF THE INVENTION

In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10] In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier. In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions. In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

[13] Methods and compositions are provided for modeling the structure of a soluble (extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding. In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure. The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis. Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor. This information provides a basis for rational drug design.

These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

DETAILED DESCRIPTION OF THE EMBODIMENTS

Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor. Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission. The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions. In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

[17]

The subject methods are useful for both prophylactic and therapeutic purposes. Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition. The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention. Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important. Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia. Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

Among gluten proteins with potential harmful effect to Celiac Sprue patients are [22] included the storage proteins of wheat, species of which include Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskyi; etc. A review of the genes encoding wheat storage proteins may be found in Colot (1990) Genet Eng (N Y) 12:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of α - and γ -gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24] Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as β -alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g., α -methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPP, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, *inter alia*, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, *e.g.* by increasing steric hindrance, altering hydrophilicity or hydrophobicity, *etc.* Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, *e.g.* by incorporating amino acids known to interact strongly with the binding cleft.

One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX₁ELX₂Y, where X_1 and X_2 are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X_1 and X_2 is a residue other than proline.

Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, *e.g.* as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, *etc.* The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35] Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones *et al.* (1991) Acta Cryst. **A47**:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger *et al.* (1998) Acta Cryst. **D54**:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack *et al.* (1997) Folding & Design **2**:27-42.

[36] It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41] The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moieties.

Computer-based methods of analysis fall into two broad classes: database methods [42] and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g. data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atomby-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker *et al.* (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell *et al.*, (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolla, Calif.); and DOCK (Kuntz *et al.* (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett *et al.* (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified. In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage. A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized *de novo*. The *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50] The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

[52] For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, e.g. by the addition of metal ions such as Mn²⁺, Pb²⁺, etc. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, e.g. by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique. Model building is facilitated by the use of sequence markers, especially selenomethionine residues. Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288). Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones et al., supra.) Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493). Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process. The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

HLA-DQ2/peptide complex structure models and databases of structure information are provided. The structural models find use in determining the structure of related and/or analogous peptide complexes. In some cases, modeling will be based on the provided structure. In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

The structure model may be implemented in hardware or software, or a combination of both. For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape. This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above. Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium. Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, corn starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz et al. (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh et al. (2001) J Control Release 71(3):307-18.

Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

METHODS OF TREATMENT

The subject methods are used to treat individuals suffering from Celiac Sprue and/or dermatitis herpetiformis, by administering an effective dose through a pharmaceutical formulation. Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art. A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease. Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] are indicative of a susceptibility to the disease. Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity. Methods for the delivery of peptides that are altered from a native peptide are known in the art. Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests. Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

Various methods for administration may be employed. The dosage of the [72] therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like. Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor. A typical dose is at least about 1 μg , usually at least about 10 μg , more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue. Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration. The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, etc. to maintain an effective dosage level.

The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM). IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk. Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, e.g. i.v., i.m., etc. Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

EXPERIMENTAL

Example

It has long been known that the principal toxic components of wheat gluten are a family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α-gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with submicromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant $\alpha 2$ -gliadin: $\alpha 2$ -gliadin, a representative α -gliadin (Arentz-Hansen et al. (2000) Gut **46**:46), was expressed in recombinant form and purified from E. coli. The $\alpha 2$ -gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μ g/ml of

kanamycin at 37 °C until the OD600 0.6-1 was achieved. The expression of α 2-gliadin protein was induced with the addition of 0.4 mM isopropyl α -D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant $\alpha 2$ -gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT; 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing $\alpha 2$ -gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and α 2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing α 2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min, rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α -2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reversephase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLCgrade acetonitrile/isopropanol: 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30-100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

	33-mer	Control A	Control B
H1P0	<20%	>90%	>90%
H2P0	<20%	>61%	>85%
H3P0	<20%	>87%	>95%
H4P0	<20%	>96%	>95%
H5P0	<20%	>96%	>95%

The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α 2-gliadin,

To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of $\alpha 2$ gliadin was then examined. As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity). In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

The small intestinal brush-border membrane (BBM) enzymes are known to be vital for breaking down any remaining peptides from gastric/pancreatic digestion into amino acids, dipeptides or tripeptides for nutritional uptake. Therefore a comprehensive analysis of gliadin metabolism also required investigations into BBM processing of gliadin peptides of reasonable length derived from gastric and pancreatic protease treatment. BBM fractions were prepared from rat small intestinal mucosa. The specific activities of known BBM peptidases were verified to be within the previously reported range. Whereas the half-life of disappearance of WQIPEQSR was ~60 min in the presence of 12 ng/µl BBM protein, the half-life of LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPP digestion was >20 h. Therefore, the latter peptide remains intact throughout the digestive process in the stomach and upper small intestine, and is poised to act as a potential antigen for T cell proliferation and intestinal toxicity in genetically susceptible individuals.

Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells. It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α -gliadin

Structural characteristics of the 33-mer gliadin peptide and its naturally occurring [81] homologs: Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire α 2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer α2-gliadin peptide are QPQPFPPQLPYPQTQPFPPQQPYPQPQPQPQPQPQ (from α 1- and α 6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from γ-gliadin); VQWPQQQPVPQPHQPF (from γ -gliadin), VQGQGIIQPQQPAQ (from γ -gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from γ -gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from γ -gliadin), QPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from ω-secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins. Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function. In both cases available information suggested that the homology could have biologically relevance. For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein. In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi. In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

Example 3

[83] X-ray Crystallographic Analysis of soluble HLA-DQ2. The soluble extracellular domains of the α - and β -chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered α - and β -chains is provided in SEQ ID NO:1 and SEQ ID NO:2. The β -chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end. Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends. Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

[84]

Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column. Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2 μ L of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2 μ L of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature. Small crystals appeared within three days and grew to full size in two weeks.

[85] For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen. X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using σ_A -weighted F_o - F_c and $2F_o$ - F_c electron density maps with the program O. The current model has R-factor of 0.2209 with a $R_{\rm free}$ of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex, α -chain of DQ2, β -chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex, α -chain, β -chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

[89] Structure-based design of DQ2 binding peptide inhibitors. The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

[90] The coordinate of the structure are as follows:

Coordinates

REMARK peptide lin	nk removed	(appli	ed DPI	EP): fro	om B	105	to B	113
REMARK peptide lin	nk removed	(appli	ed DPI	EP): fro	om E	104	to E	113
REMARK disulphide				to A	163			
REMARK disulphide	added: from	n B	15	to B	79			
REMARK disulphide	added: from	n B	117	to B	173			

163

107 to D

REMARK disulphide added: from D

REMARK	_	-					15		E	79			
REMARK	_	•								173			
		•								by user:	kim		
REMARK		-								•			
MOTA	1	CB	VAL	A	2	31	.060	3	8.851	4.095	1.00	39.43	A
MOTA	2	CG1	VAL	A	2	30	.078	2	2.835	3.531	1.00	40.06	A
ATOM	3	CG2	VAL	A	2	30	.370	5	.185	4.344	1.00	39.97	\mathbf{A}
MOTA	4	C	VAL	A	2	30	.653	3	3.406	6.542	1.00	36.80	A
MOTA	5	0	VAL	A	2	29	.644		2.702			38.25	A
MOTA	6	N	VAL	A	2	32	.189	1	1.926			36.80	A
ATOM	7	CA	VAL		2		.684		3.321			37.95	A
ATOM	8	N	ALA		3		.910		.267			34.99	
ATOM	9	CA	ALA		3		.003		1.416			32.94	A
MOTA	10	CB	ALA		3		.325		3.368			33.34	A
ATOM	11	C	ALA		3		.094		5.805			30.81	A
ATOM	12	0	ALA		3		.980		5.583			29.57 28.70	A A
ATOM	13	N	ASP		4 4		.172 .173		7.416			26.95	A
ATOM	14 15	CA CB	ASP ASP		4		.812		7.722			28.65	A
ATOM ATOM	15 16	CG	ASP		4		.687		7.845			31.67	
ATOM	17		ASP		4		.904		3.417			33.31	A
ATOM	18		ASP		4		.568		7.381			33.31	A
ATOM	19	C	ASP		4		.254		7.432			26.51	A
ATOM	20	0	ASP		4		.857		3.469			25.25	A
ATOM	21	N	HIS		5		.493		5.277			26.22	A
ATOM	22	CA	HIS		5	31	.527	e	5.164	13.544	1.00	26.52	A
ATOM	23	CB	HIS	A	5	30	.939	E	3.339	14.950	1.00	25.34	A
MOTA	24	CG	HIS	A	5	30	.240	-	7.647	15.156	1.00	28.69	A
ATOM	25	CD2	HIS	A	5	30	.716	8	3.870	15.492	1.00	29.15	A
MOTA	26	ND1	HIS	A	5	28	.881	7	7.801	14.979	1.00	28.23	A
MOTA	27	CE1	HIS	A	5	28	.550	9	9.062	15.198	1.00	29.92	A
ATOM	28	NĖ2	HIS	A	5	29	.645		732				A
MOTA	29	C	HIS		5		.246		1.826		1.00	25.79	A
ATOM	30	0	HIS		5		.630		3.785		1.00		A
ATOM	31	N	VAL		6		.559		1.866			24.52	A
ATOM	32	CA	VAL		6		.385		3.667				A
ATOM	33	CB	VAL		6		.311		3.657				A
ATOM	34	CG1	VAL		6 6		.187 .489		2.414 3.708		1.00		A A
ATOM	35 36	CG2 C	VAL VAL		6		.409 .256		3.633				A
ATOM ATOM	36 37	0	VAL		6		.230 .937		1.606				A
ATOM	38	Ŋ	ALA		7		.239		2.513				A
ATOM	39	CA	ALA		7		.038		2.382				A
ATOM	40	CB	ALA		7		.132		2.394				A
ATOM	41	C	ALA		7		.867		1.111				A
ATOM	42	0	ALA		7		.548		0.153			20.78	A
ATOM	43	N	SER		8		.947		1.120	17.560	1.00	16.95	A
ATOM	44	CA	SER	A	8	38	.807	- (0.048	17.700	1.00	18.62	A
ATOM	45	CB	SER	A	8	40	.211	(0.215	17.153	1.00	17.69	A
ATOM	46	OG	SER	A	8	40	.209	(0.271	15,738	1.00	19.81	A
MOTA	47	C	SER	A	8	38	.868	- (0.310	19.199		18.76	A
MOTA	48	0	SER		8		.570		0.376			19.35	A
MOTA	49	N	TYR		9		.070		1.268				A
ATOM	50	CA	TYR		9		.038		1.608			19.44	A
ATOM	51	CB	TYR		9		.628		1.980				A
ATOM	52	CG	TYR		9		.714		0.785				A A
ATOM	53 54	CD1			9 9		.073		0.435 1.537			17.39	A
ATOM ATOM	54 55	CD2	TYR TYR		9		.493		0.865			17.15	A
ATOM	55 56	CE2			9		.641		0.003 0.235				A
ATOM	57	CEZ	TYR		9		.020		1.431				A
ATOM	58	OH	TYR		9		.169		2.509				A
ATOM	59	C	TYR		9		.993		2.751				A
ATOM	60	o	TYR		9		.652		3.911				A
ATOM	61	N	GLY		10		.225		2.357			21.69	A
ATOM	62	CA	GLY		10	41	.311	:	3.275	20.808	1.00	22.54	A
MOTA	63	C	GLY	A	10	42	.276	-:	3.080	19.655	1.00	21.74	A
ATOM	64	0	GLY	A	10		.248		3.863				A
MOTA	65	N	VAL	A	11		.083		2.023				A
ATOM	66	CA	VAL		11		.119		1.949				A
ATOM	67	CB	VAL		11		.554		0.506				A
ATOM	68	CG1			11		.845		0.558				A
ATOM	69	CG2	VAL	A	11	43	.481	•	0.165	17.432	1.00	15.25	A

ATOM	70	С	VAL	A	11	45.228	-2.644	19.447	1.00 17.05	A
ATOM	71	0	VAL	A	11	45.679	-2.145	20.481	1.00 19.34	A
ATOM	72	N	ASN		12	45.616	-3.828	19.005	1.00 17.39	A .
ATOM	73	CA	ASN		12	46.643	-4.597	19.693	1.00 17.18	A
ATOM	74	CB	ASN		12	46.113 44.834	-5.994 -5.947	20.052	1.00 15.04 1.00 15.96	A A
ATOM ATOM	75 76	CG OD1	ASN ASN		12 12	43.780	-5.490	20.882	1.00 18.20	A
ATOM	77	ND2	ASN		12	44.921	-6.420	22.114	1.00 10.46	A
ATOM	78	C	ASN		12	47.863	-4.739	18.797	1.00 18.90	A
ATOM	79	0	ASN		12	47.752	-5.162	17.641	1.00 18.80	A
ATOM	80	N	LEU	A	13	49.026	-4.403	19.343	1.00 18.60	A
ATOM	81	CA	LEU	A	13	50.264	-4.478	18.599	1.00 19.90	A
ATOM	82	CB		A	13	50.695	-3.064	18.217	1.00 23.26	A
ATOM	83	CG		A	13	52.077	-2.881	17.594	1.00 24.86	A
ATOM	84	CD1		A	13	52.085	-3.494 -1.402	16.201 17.534	1.00 26.92 1.00 24.75	A A
ATOM ATOM	85 86	CD2 C	LEU LEU		13 13	52.417 51.391	-1.40 <i>2</i> -5.165	19.370	1.00 24.73	A
ATOM	87	0	LEU		13	51.559	-4.953	20.566	1.00 21.11	A
ATOM	88	N	TYR		14	52.145	-6.004	18.673	1.00 21.04	A
ATOM	89	CA	TYR	A	14	53.291	-6.691	19.255	1.00 24.07	A
ATOM	90	CB	TYR	A	14	52.909	-8.050	19.844	1.00 27.05	A
ATOM	91	CG	TYR	Α	14	54.091	-8.729	20.489	1.00 29.27	A
ATOM	92	CD1	TYR		14	54.569	-8.304	21.723	1.00 30.07	A
ATOM	93	CE1	TYR		14	55.709	-8.867	22.285	1.00 31.38	A
MOTA	94	CD2			14	54.783	-9.744 -10.314	19.830 20.383	1.00 31.63 1.00 30.29	A A
ATOM ATOM	95 96	CE2 CZ	TYR TYR		14 14	55.923 56.381	-9.868	20.363	1.00 30.25	A
ATOM	97	OH	TYR		14		-10.413	22.160	1.00 34.48	A
ATOM	98	C	TYR		14	54.291	-6.900	18.128	1.00 25.30	A
ATOM	99	0	TYR		14	53.907	-7.206	16.994	1.00 25.51	A
ATOM	100	N	GLN	A	15	55.571	-6.725	18.429	1.00 24.61	A
ATOM	101	CA	GLN	A	15	56.603	-6.891	17.414	1.00 25.19	A
MOTA	102	CB	GLN	A	15	56.932	-5.549	16.754	1.00 23.54	A
MOTA	103	CG	GLN		15	57.278	-4.443	17.738	1.00 23.98	A
ATOM	104	CD	GLN		15	57.567	-3.116	17.056	1.00 26.32	A A
ATOM	105	OE1			15 15	57.575 57.810	-2.062 -3.159	17.702 15.749	1.00 28.26 1.00 24.64	A
ATOM ATOM	106 107	NE2 C	GLN GLN		15 15	57.848	-7.487	18.036	1.00 24.04	A
ATOM	108	0	GLN		15	58.134	-7.263	19.211	1.00 24.31	A
ATOM	109	N	SER		16	58.583	-8.252	17.236	1.00 28.72	A
ATOM	110	CA	SER		16	59.801	-8.912	17.698	1.00 30.37	A
ATOM	111	CB	SER	A	16	60.341	-9.830	16.603	1.00 28.35	A
ATOM	112	OG	SER	A	16	60.569	-9.100	15.407	1.00 31.43	A
ATOM	113	C	SER		16	60.883	-7.918	18.111	1.00 32.37	A
ATOM	114	0	SER		16	61.538	-8.104	19.134	1.00 33.91 1.00 32.49	A A
ATOM	115	N	TYR TYR		17 17	61.073 62.096	-6.863 -5.890	17.325 17.664	1.00 32.49	A
ATOM ATOM	116 117	CA CB	TYR		17	62.030	-4.788	16.620	1.00 35.41	A
ATOM	118	CG	TYR		17	63.371	-3.911	16.837	1.00 37.77	A
ATOM	119	CD1			17	64.646	-4.347	16.470	1.00 39.38	A
ATOM	120	CE1			17	65.769	-3.569	16.715	1.00 40.15	A
ATOM	121	CD2	TYR	A	17	63.247	-2.671	17.456	1.00 36.31	A
ATOM	122	CE2			17	64.360	-1.886	17.707	1.00 39.40	A
MOTA	123	CZ	TYR		17	65.621	-2.338	17.335	1.00 41.42	A
ATOM	124	OH	TYR		17	66.732	-1.562	17.580	1.00 43.02 1.00 34.43	A A
ATOM	125	C	TYR		17 17	61.821 60.765	-5.270 -4.682	19.027 19.248	1.00 34.43	Ā
ATOM ATOM	126 127	И	TYR GLY		1.8	62.783	-5.390	19.240	1.00 33.30	A
ATOM	128	CA	GLY		18	62.609	-4.854	21.270	1.00 35.78	A
ATOM	129	C	GLY		18	62.730	-5.968	22.292	1.00 36.87	A
ATOM	130	Ō	GLY		18	63.761	-6.082	22.952	1.00 38.48	A
ATOM	131	N	PRO	A	19	61.692	-6.807	22.459	1.00 37.06	A
ATOM	132	CD	PRO	A	19	61.745	-7.967	23.368	1.00 35.58	A
MOTA	133	CA	PRO		19	60.409	-6.769	21.747	1.00 34.79	A
ATOM	134	CB	PRO		19	59.853	-8.166	21.981	1.00 35.91	A N
ATOM	135	CG	PRO		19 10	60.300	-8.437	23.394	1.00 36.88 1.00 33.10	A A
ATOM	136	C	PRO		19 19	59.531 59.844	-5.706 -5.209	22.379 23.456	1.00 33.10	A
ATOM ATOM	137 138	O N	PRO SER		20	58.435	-5.349	23.436	1.00 33.71	A
ATOM	139	CA	SER		20	57.548	-4.341	22.290	1.00 30.25	A
ATOM	140	CB	SER		20	58.060	-2.932	21.965	1.00 29.00	A '
MOTA	141	OG	SER		20	58.072	-2.689	20.567	1.00 32.27	A
ATOM	142	C	SER		20	56.108	-4.497	21.820	1.00 27.93	A
MOTA	143	0	SER	A	20	55.829	-5.129	20.805	1.00 28.23	A
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ATOM	144	N	GLY		21	55.191	-3.911 -4.001	22.576	1.00 25.87 1.00 23.78	A A
ATOM ATOM	145 146	CA C	GLY GLY		21 21	53.797 53.076	-4.001 -2.732	22.598	1.00 23.76	A
ATOM	147	0	GLY		21	53.638	-1.840	23.247	1.00 24.81	A
ATOM	148	N	GLN		22	51.821	-2.641	22.187	1.00 20.60	A
ATOM	149	CA	GLN	A	22	51.033	-1.470	22.495	1.00 19.67	A
ATOM	150	CB	GLN		22	51.239	-0.400	21.415	1.00 19.28	A
ATOM	151	CG	GLN		22	50.584	0.943 1.971	21.736 20.613	1.00 18.12 1.00 18.84	A A
ATOM	152	CD OE1	GLN GLN		22 22	50.732 51.694	2.749	20.515	1.00 10.04	A
ATOM ATOM	153 154	NE2	GLN		22	49.777	1.968	19.688	1.00 16.83	A
ATOM	155	C	GLN		22	49.573	-1.873	22.566	1.00 18.66	A
ATOM	156	0	GLN	A	22	49.128	-2.747	21.826	1.00 18.45	A
ATOM	157	N	TYR	A	23	48.842	-1.257	23.484	1.00 17.25	A
ATOM	158	CA	TYR		23	47.423	-1.529	23.615 24.752	1.00 16.53 1.00 14.51	A A
ATOM	159	CB CG	TYR TYR		23 23	47.127 45.674	-2.497 -2.904	24.752	1.00 12.67	A
ATOM ATOM	160 161	CD1	TYR		23	45.251	-4.070	24.121	1.00 13.38	A
ATOM	162	CE1	TYR		23	43.904	-4.415	24.070	1.00 13.23	A
MOTA	163	CD2	TYR	A	23	44.713	-2.093	25.346	1.00 11.07	A
MOTA	164	CE2	TYR		23	43.365	-2.425	25.299	1.00 12.99	A A
MOTA	165	CZ	TYR		23	42.964 41.624	-3.583 -3.907	24.664 24.611	1.00 13.72 1.00 17.15	A
MOTA	166 167	OH C	TYR TYR		23 23	46.694	-0.220	23.860	1.00 16.88	A
ATOM ATOM	168	0	TYR		23	46.975	0.491	24.824	1.00 16.57	A
ATOM	169	N	THR		24	45.757	0.085	22.969	1.00 16.16	A
MOTA	170	CA	THR	. A	24	44.975	1.311	23.038	1.00 16.43	A
MOTA	171	CB	THR		24	45.594	2.405	22.136	1.00 18.41 1.00 17.20	A A
ATOM	172	OG1			24	45.581 47.029	1.954 2.692	20.771 22.537	1.00 17.20	A
ATOM ATOM	173 174	CG2 C	THR		24 24	43.570	1.058	22.499	1.00 15.15	A
ATOM	175	0	THR		24	43.314	0.037	21.879	1.00 15.70	A
ATOM	176	N	HIS	A	25	42.667	1.993	22.754	1.00 15.66	A
MOTA	177	CA	HIS		25	41.320	1.924	22.210	1.00 15.79	A
MOTA	178	CB	HIS		25	40.243	1.834 0.430	23.297 23.734	1.00 13.55 1.00 15.91	A A
MOTA	179	CG CD2	HIS HIS		25 25	39.956 40.688	-0.704	23.624	1.00 13.86	A
ATOM ATOM	180 181	ND1			25	38.790	0.071	24.374	1.00 15.91	A
MOTA	182	CE1			25	38.815	-1.222	24.639	1.00 14.38	A
ATOM	183	NE2	HIS	A	25	39.956	-1.715	24.193	1.00 16.99	A
MOTA	184	C	HIS		25	41.176	3.212	21.437 21.865	1.00 14.18 1.00 13.52	A A
ATOM	185	O N	HIS GLU		25 26	41.677 40.510	4.241 3.150	20.292	1.00 13.32	A
ATOM ATOM	186 187	N CA	GLU		26	40.333	4.329	19.462	1.00 16.96	A
ATOM	188	CB		JA	26	41.132	4.188	18.164	1.00 16.34	A
ATOM	189	CG	GLU	JA	26	42.644	4.158	18.311	1.00 18.80	A
ATOM	190	CD		JA	26	43.345	4.036	16.958	1.00 22.68	A A
ATOM	191	OE1	_	JA	26 26	42.744	4.456 3.539	15.946 16.901	1.00 26.77 1.00 20.46	A
ATOM ATOM	192 193	OE2		JA JA	26 26	44.490 38.875	4.543	19.101	1.00 17.22	A
ATOM	194	0		JA		38.104	3.597	18.996	1.00 18.66	A
ATOM	195	N	PHI	EΑ	27	38.503	5.802		1.00 18.91	A
MOTA	196	CA		E A		37.150	6.135	18.509	1.00 19.32	A.
MOTA	197	CB		E A		36.290	6.546 6.653	19.698 19.357	1.00 20.19 1.00 23.33	A A
ATOM	198			E A E A		34.834 34.024			1.00 22.07	A
ATOM ATOM	199 200			E A		34.289			1.00 23.24	A
ATOM	201	CE:	_	ΕA		32.692	5.606	18.980	1.00 26.16	A
ATOM	202	CE	2 PH	E A		32.954			1.00 25.99	A
MOTA	203			E A		32.155			1.00 25.46 1.00 19.10	A A
ATOM	204			E A E A		37.260 37.733			1.00 19.83	A
MOTA MOTA	205 206			r A P A		36.831				A
ATOM	200			PA		36.901	_		1.00 18.94	A
ATOM	208			P A	. 28	35.910	9.203			A
MOTA	209			P A		34.472				A z
ATOM	210		1 AS			34.266				A A
MOTA	211		2 AS	PA		33.552 38.297				A
MOTA MOTA	212 213			PA		38.467				A
ATOM	214			Y A		39.292	_	15.002		A
ATOM	215			Y A		40.658				A.
ATOM	216			Y A		41.437				A A
MOTA	217	0	GL	Y A	A 29	42.621			J. 00 LJ. 20	£.3*
								96		

ATOM 219 CA ASP A 30 41.511 9.438 18.254 1.00 16.83 A ATOM 220 CB ASP A 30 40.816 10.678 18.796 1.00 18.99 A ATOM 221 CG ASP A 30 40.988 11.864 17.888 1.00 21.09 A ATOM 222 OD1 ASP A 30 42.145 12.177 17.538 1.00 22.94 A ATOM 223 OD2 ASP A 30 42.145 12.177 17.538 1.00 22.94 A ATOM 224 C ASP A 30 41.656 8.392 19.345 1.00 17.25 A ATOM 225 O ASP A 30 40.777 7.553 19.545 1.00 15.40 A ATOM 226 N GLU A 31 42.784 8.453 20.041 1.00 16.77 A ATOM 227 CA GLU A 31 43.111 7.514 21.107 1.00 18.43 A ATOM 228 CB GLU A 31 44.620 7.607 21.392 1.00 20.90 A ATOM 229 CG GLU A 31 45.147 6.853 22.608 1.00 24.68 A ATOM 230 CD GLU A 31 46.678 6.924 22.702 1.00 27.25 A ATOM 231 OE1 GLU A 31 47.258 7.931 22.239 1.00 26.93 A ATOM 233 C GLU A 31 47.258 7.931 22.239 1.00 27.21 A ATOM 233 C GLU A 31 47.302 5.985 23.242 1.00 27.21 A ATOM 233 C GLU A 31 42.296 7.777 22.375 1.00 17.51 A ATOM 234 O GLU A 31 42.361 8.863 22.952 1.00 17.51 A ATOM 235 N GLU A 32 41.525 6.784 22.807 1.00 15.91 A ATOM 236 CA GLU A 32 41.525 6.784 22.807 1.00 15.91 A ATOM 237 CB GLU A 32 39.542 5.980 24.020 1.00 15.91 A ATOM 237 CB GLU A 32 39.542 5.980 24.020 1.00 15.91 A ATOM 238 CG GLU A 32 39.542 5.980 24.020 1.00 15.91 A ATOM 238 CG GLU A 32 39.542 5.980 24.020 1.00 15.91 A ATOM 238 CG GLU A 32 39.542 5.980 24.020 1.00 15.91 A ATOM 238 CG GLU A 32 39.542 5.980 24.020 1.00 15.97 A ATOM 238 CG GLU A 32 39.542 5.980 24.020 1.00 15.97 A ATOM 240 OE1 GLU A 32 37.478 4.228 22.808 1.00 18.09 A ATOM 240 OE1 GLU A 32 37.478 4.228 22.808 1.00 18.09 A ATOM 241 NE2 GLU A 32 37.478 4.228 22.808 1.00 15.51 A ATOM 244 N PHE A 33 42.470 5.912 23.374 1.00 20.57 A ATOM 245 CA PHE A 33 42.470 5.720 25.151 1.00 15.51 A ATOM 245 CA PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 246 CB PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 245 CA PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 246 CB PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 246 CB PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 247 CG PHE A 33 42.583 4.854 27.443 1.00 17.21 A ATOM 247 CG PHE A 33 42.583 4.854 27.443 1.00 1											
NEON 200 CB ASP A 30	ATOM	218	N	ASP	A	30	40.797	8.922	17.098		
NECON 221	ATOM	219	CA	ASP	A	30	41.511				
NEW 1976 1	MOTA	220	CB	ASP	A	30	40.816				
NATION 223 ODE ARP A 30 39.971 12.478 17.525 1.00 21.68 A	ATOM	221									
NEON 224 C	ATOM	222									
NECON 225	ATOM	223									
NOON	ATOM										
NEON	ATOM										
ATOM 298 CB GLU A 31	ATOM										
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AROM 241 NEZ GLN A 32 36.091 5.912 23.374 1.00 20.57 A RITOM 242 C GLN A 32 41.594 6.701 25.255 1.00 16.61 A RITOM 243 O GLN A 32 41.594 6.701 25.255 1.00 16.51 A RITOM 244 N PHE A 33 42.470 5.720 25.151 1.00 16.634 A RITOM 246 CR PHE A 33 42.470 5.389 26.239 1.00 16.34 A RITOM 246 CR PHE A 33 42.583 4.854 27.443 1.00 17.21 A RITOM 240 CR PHE A 33 42.583 4.854 27.443 1.00 17.21 A RITOM 240 CR PHE A 33 42.583 4.854 27.443 1.00 16.56 A RITOM 240 CR PHE A 33 42.583 4.951 1.00 27.22 1.00 16.63 A RITOM 240 CR PHE A 33 42.686 2.333 27.406 1.00 16.557 A RITOM 240 CR PHE A 33 42.083 1.076 27.288 1.00 16.34 A RITOM 250 CR PHE A 33 49.083 2.147 26.903 1.00 18.54 A RITOM 250 CR PHE A 33 49.729 0.993 26.903 1.00 18.56 A RITOM 251 CR PHE A 33 49.729 0.993 26.903 1.00 16.34 A RITOM 250 CR PHE A 33 49.729 0.993 26.978 1.00 16.56 A RITOM 250 CR PHE A 33 44.363 4.343 25.776 1.00 16.66 A RITOM 250 CR PHE A 33 44.363 4.343 25.776 1.00 16.66 A RITOM 250 CR PHE A 33 44.363 4.343 25.776 1.00 16.66 A RITOM 250 CR PHE A 34 46.377 3.125 26.251 1.00 16.03 A RITOM 250 CR PHE A 34 46.377 3.125 26.264 1.00 16.03 A RITOM 250 CR PHE A 34 46.377 3.125 26.264 1.00 16.03 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.38 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.38 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.38 A RITOM 250 CR PHE A 34 49.519 3.993 26.578 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.38 A RITOM 250 CR PHE A 34 49.519 3.993 26.586 1.00 17.38 A RITOM 250 CR PHE A 34 49.519 3.993 26.593 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 26.593 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 26.593 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.48 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.48 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.48 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.48 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.31 A RITOM 250 CR PHE A 34 49.519 3.993 27.291 1.00 17.31 A RITOM 25	ATOM					32	37.478	4.228	22.808	1.00 18.09	
ARDOM 242 C GLN A 32 41.584 6.701 25.255 1.00 16.61 A ARDOM 243 O GLN A 32 41.448 7.387 26.272 1.00 15.59 A ARDOM 244 N PHE A 33 42.470 5.720 25.151 1.00 15.59 A ARDOM 245 CA PHE A 33 42.583 4.854 27.443 1.00 17.21 A ARDOM 246 CB PHE A 33 42.583 4.854 27.443 1.00 17.21 A ARDOM 247 CG PHE A 33 42.583 4.854 27.463 1.00 17.21 A ARDOM 247 CG PHE A 33 42.583 1.002 27.222 1.00 16.68 A ARDOM 249 CD2 PHE A 33 42.583 1.002 27.222 1.00 16.68 A ARDOM 249 CD2 PHE A 33 42.686 2.333 27.406 1.00 15.57 A ARDOM 249 CD2 PHE A 33 42.686 2.333 27.406 1.00 16.56 A ARDOM 251 CE2 PHE A 33 40.598 3.397 26.903 1.00 18.54 A ARDOM 251 CE2 PHE A 33 42.083 1.006 27.288 1.00 16.34 A ARDOM 251 CE2 PHE A 33 40.729 0.983 26.978 1.00 16.66 A ARDOM 251 CE2 PHE A 33 44.053 4.343 25.776 1.00 16.66 A ARDOM 255 C TRY A 34 45.398 4.139 26.978 1.00 16.66 A ARDOM 255 N TYR A 34 45.398 4.139 26.572 1.00 16.03 A ARDOM 256 CA TYR A 34 46.377 3.125 26.264 1.00 16.93 A ARDOM 256 CA TYR A 34 46.377 3.125 26.264 1.00 16.93 A ARDOM 256 CB TYR A 34 47.636 3.730 25.621 1.00 16.93 A ARDOM 258 CG TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 250 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 250 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 250 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 250 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.31 A ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD1 TYR A 34 49.519 3.993 27.291 1.00 17.68 ARDOM 260 CD2 TYR A 34 49.510 49.291 3.993 27.398 1.00 19.73 ARDOM 260 CD2 TYR A 34 49.519 3.993 27.398 1.00 19.76 ARDOM 260 CD2 TYR A 34 49.519 3.993 37.391 37.301 37.301 37.301 ARDOM 260 CD2 TYR A 34 49.519 3.993 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301 37.301	ATOM		NE2	GLN	A	32	36.091				A
ARDOM 244 N PHE A 33 42.647 5.7.02 25.151 1.00 15.59 A ARDOM 246 CB PHE A 33 42.670 5.702 25.151 1.00 15.59 A ARDOM 246 CB PHE A 33 42.583 42.640 5.702 25.151 1.00 16.34 A ARDOM 246 CB PHE A 33 42.583 42.646 2.333 27.406 1.00 17.21 A ARDOM 248 CD1 PHE A 33 42.686 2.333 27.406 1.00 15.57 A ARDOM 248 CD1 PHE A 33 40.598 3.397 26.903 1.00 18.54 A ARDOM 249 CD2 PHE A 33 40.598 3.397 26.903 1.00 18.54 A ARDOM 250 CE1 PHE A 33 40.598 3.397 26.903 1.00 16.34 A ARDOM 251 CE2 PHE A 33 40.729 0.983 26.978 1.00 16.34 A ARDOM 251 CE2 PHE A 33 40.729 0.983 26.978 1.00 16.34 A ARDOM 252 CZ PHE A 33 40.729 0.983 26.978 1.00 16.56 A ARDOM 253 C PHE A 33 44.363 25.776 1.00 16.56 A ARDOM 253 C PHE A 33 44.363 25.776 1.00 16.66 A ARDOM 255 N TYR A 34 44.5398 4.139 26.572 1.00 16.68 A ARDOM 255 N TYR A 34 46.377 3.125 26.264 1.00 16.93 ARDOM 256 CA TYR A 34 46.377 3.125 26.264 1.00 16.93 ARDOM 257 CB TYR A 34 49.519 3.930 27.291 1.00 16.93 ARDOM 259 CD1 TYR A 34 49.519 3.930 27.291 1.00 17.31 ARDOM 259 CD1 TYR A 34 49.519 3.930 27.291 1.00 17.31 ARDOM 250 CD1 TYR A 34 49.519 3.930 27.291 1.00 17.31 ARDOM 250 CD1 TYR A 34 49.519 3.930 27.291 1.00 17.38 ARDOM 260 CE1 TYR A 34 49.244 6.690 27.388 1.00 17.31 ARDOM 261 CD2 TYR A 34 48.504 5.932 26.586 1.00 17.68 ARDOM 263 CZ TYR A 34 48.504 5.932 27.291 1.00 17.48 ARDOM 264 CH2 TYR A 34 48.504 5.932 27.291 1.00 17.48 ARDOM 265 C TYR A 34 48.504 5.932 27.291 1.00 17.48 ARDOM 266 CB1 TYR A 34 48.504 5.932 27.291 1.00 17.31 ARDOM 266 CB2 TYR A 34 48.504 5.932 27.291 1.00 17.31 ARDOM 267 N VAL A 35 46.692 2.473 27.588 1.00 17.31 ARDOM 268 C TYR A 34 48.504 5.932 27.291 1.00 17.68 ARDOM 267 N VAL A 35 47.513 1.261 27.555 1.00 17.31 ARDOM 268 C TYR A 34 46.692 2.473 27.588 1.00 17.68 ARDOM 267 N VAL A 35 47.513 1.261 27.555 1.00 17.31 ARDOM 267 N VAL A 35 47.513 1.261 27.555 1.00 17.31 ARDOM 268 C TYR A 34 46.692 2.473 27.291 1.00 17.68 ARDOM 267 N VAL A 35 47.513 1.261 27.555 1.00 17.31 ARDOM 268 C TYR A 36 51.544 1.122 29.048 1.00 19.75 ARDOM 277 C TYR A 36 51.546 1.00 18.89 ARDOM 277 C TY	ATOM		C	GLN	A	32					
ARTOM 245 CA PHE A 33	MOTA	243	0	GLN	A	32					
ATOM 246 CB PHE A 33	MOTA	244	N	PHE	A	33					
ATOM 247 CG PHE A 33	ATOM	245	CA	PHE	A	33					
ATOM 248 CD1 PHE A 33	MOTA	246									
ATOM 249 CD2 PHE A 33	MOTA										
ATOM 250 CEL PHE A 33	ATOM										
ATOM 251 CE2 PHE A 33											
ATOM 252 CZ PHE A 33											
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ATOM 264 OH TYR A 34 51.044 6.815 28.941 1.00 23.02 A ATOM 265 C TYR A 34 46.692 2.473 27.588 1.00 17.88 A ATOM 266 O TYR A 34 46.692 3.042 28.646 1.00 21.13 A ATOM 267 N VAL A 35 47.213 1.261 27.535 1.00 17.31 A ATOM 268 CA VAL A 35 47.571 0.570 28.749 1.00 18.89 A ATOM 269 CB VAL A 35 46.950 -0.848 28.804 1.00 19.12 A ATOM 270 CG1 VAL A 35 45.454 -0.742 29.048 1.00 19.75 A ATOM 271 CG2 VAL A 35 45.454 -0.742 29.048 1.00 19.75 A ATOM 273 O VAL A 35 49.084 0.478 28.786 1.00 18.84 A ATOM 273 O VAL A 35 49.701 -0.050 27.877 1.00 16.51 A ATOM 274 N ASP A 36 51.121 0.984 29.996 1.00 22.55 A ATOM 275 CA ASP A 36 51.542 1.872 31.172 1.00 25.86 A ATOM 276 CB ASP A 36 53.033 2.108 31.221 1.00 26.55 A ATOM 277 CG ASP A 36 53.033 2.108 31.221 1.00 26.55 A ATOM 279 OD2 ASP A 36 51.393 -0.484 30.314 1.00 29.78 A ATOM 280 C ASP A 36 51.016 -0.976 31.378 1.00 27.38 A ATOM 281 O ASP A 36 51.016 -0.976 31.378 1.00 27.38 A ATOM 282 N LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 284 CB LEU A 37 52.024 -1.187 29.387 1.00 25.10 A ATOM 285 CG LEU A 37 52.024 -1.187 29.387 1.00 25.10 A ATOM 286 CD1 LEU A 37 52.024 -1.187 29.387 1.00 25.10 A ATOM 287 CD2 LEU A 37 52.025 -3.630 25.852 1.00 21.32 A ATOM 288 C LEU A 37 52.265 -3.630 25.852 1.00 21.32 A ATOM 288 C D LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 31.43 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 31.43 A			CZ	TYR	A	34	50.224	6.060	28.141	1.00 20.10	A
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ATOM 266 O TYR A 34 46.429 3.042 28.646 1.00 21.13 A ATOM 267 N VAL A 35 47.213 1.261 27.535 1.00 17.31 A ATOM 268 CA VAL A 35 47.571 0.570 28.749 1.00 18.89 A ATOM 269 CB VAL A 35 46.950 -0.848 28.804 1.00 19.12 A ATOM 270 CG1 VAL A 35 47.589 -1.660 29.912 1.00 17.56 A ATOM 271 CG2 VAL A 35 45.454 -0.742 29.048 1.00 19.75 A ATOM 272 C VAL A 35 49.084 0.478 28.786 1.00 18.84 A ATOM 273 O VAL A 35 49.084 0.478 28.786 1.00 18.84 A ATOM 274 N ASP A 36 49.676 1.039 29.830 1.00 22.55 A ATOM 275 CA ASP A 36 51.121 0.984 29.996 1.00 25.86 A ATOM 276 CB ASP A 36 51.542 1.872 31.172 1.00 26.89 A ATOM 277 CG ASP A 36 53.033 2.108 31.221 1.00 26.55 A ATOM 278 OD1 ASP A 36 53.441 3.285 31.213 1.00 30.03 A ATOM 279 OD2 ASP A 36 51.393 -0.484 30.314 1.00 29.78 A ATOM 280 C ASP A 36 51.393 -0.484 30.314 1.00 27.38 A ATOM 281 O ASP A 36 51.016 -0.976 31.378 1.00 27.38 A ATOM 282 N LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 283 CA LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 284 CB LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 285 CG LEU A 37 52.024 -3.231 28.270 1.00 29.51 A ATOM 286 CD1 LEU A 37 52.024 -3.231 28.270 1.00 29.51 A ATOM 287 CD2 LEU A 37 52.024 -3.231 28.270 1.00 25.10 A ATOM 288 C LEU A 37 52.265 -3.630 25.852 1.00 21.32 A ATOM 288 C LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.348 -2.838 30.674 1.00 30.95 A			C	TYR	A S	34	46.692	2.473			
ATOM 268 CA VAL A 35			0	TYR	A S	34					
ATOM 269 CB VAL A 35		267	N	VAI	A						
ATOM 270 CG1 VAL A 35 47.589 -1.660 29.912 1.00 17.56 A ATOM 271 CG2 VAL A 35 45.454 -0.742 29.048 1.00 19.75 A ATOM 272 C VAL A 35 49.084 0.478 28.786 1.00 18.84 A ATOM 273 O VAL A 35 49.701 -0.050 27.877 1.00 16.51 A ATOM 274 N ASP A 36 49.676 1.039 29.830 1.00 22.55 A ATOM 275 CA ASP A 36 51.121 0.984 29.996 1.00 25.86 A ATOM 276 CB ASP A 36 51.542 1.872 31.172 1.00 26.89 A ATOM 277 CG ASP A 36 53.033 2.108 31.221 1.00 26.55 A ATOM 278 OD1 ASP A 36 53.796 1.125 31.270 1.00 29.78 A ATOM 279 OD2 ASP A 36 53.441 3.285 31.213 1.00 30.03 A ATOM 280 C ASP A 36 51.393 -0.484 30.314 1.00 26.39 A ATOM 281 O ASP A 36 51.016 -0.976 31.378 1.00 27.38 A ATOM 282 N LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 283 CA LEU A 37 52.305 -2.600 29.588 1.00 29.51 A ATOM 284 CB LEU A 37 52.754 -3.231 28.270 1.00 26.29 A ATOM 285 CG LEU A 37 52.754 -3.231 28.270 1.00 26.59 A ATOM 286 CD1 LEU A 37 52.265 -3.630 25.852 1.00 21.32 A ATOM 287 CD2 LEU A 37 50.455 -3.876 27.557 1.00 22.51 A ATOM 288 C LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 31.43 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 31.43 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 33.46 A	MOTA	268	CA	IAV	A	35					
ATOM 271 CG2 VAL A 35	MOTA	269	CB								
ATOM 271 CG VAL A 35	MOTA	270									
ATOM 273 O VAL A 35	MOTA										
ATOM 274 N ASP A 36											
ATOM 275 CA ASP A 36 51.121 0.984 29.996 1.00 25.86 A ATOM 276 CB ASP A 36 51.542 1.872 31.172 1.00 26.89 A ATOM 277 CG ASP A 36 53.033 2.108 31.221 1.00 26.55 A ATOM 278 OD1 ASP A 36 53.796 1.125 31.270 1.00 29.78 A ATOM 279 OD2 ASP A 36 53.441 3.285 31.213 1.00 30.03 A ATOM 280 C ASP A 36 51.393 -0.484 30.314 1.00 26.39 A ATOM 281 O ASP A 36 51.016 -0.976 31.378 1.00 27.38 A ATOM 282 N LEU A 37 52.024 -1.187 29.387 1.00 27.51 A ATOM 283 CA LEU A 37 52.305 -2.600 29.588 1.00 29.51 A ATOM 284 CB LEU A 37 52.754 -3.231 28.270 1.00 26.29 A ATOM 285 CG LEU A 37 52.265 -3.630 25.852 1.00 21.32 A ATOM 287 CD2 LEU A 37 50.455 -3.876 27.557 1.00 22.51 A ATOM 288 C LEU A 37 53.348 -2.838 30.674 1.00 30.95 A ATOM 289 O LEU A 37 53.222 -3.774 31.457 1.00 31.43 A ATOM 289 O LEU A 38 54.362 -1.980 30.734 1.00 33.46 A ATOM 290 N GLY A 38 54.362 -1.980 30.734 1.00 33.46 A											
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ATOM 290 N GLY A 38 54.362 -1.980 30.734 1.00 33.46 A											A
THE TOTAL TO									30.734	1.00 33.46	A
							55.403	-2.140	31.737	1.00 35.44	A

MOTA	292	C	GLY	A	38	54.956	-1.863	33.162	1.00 37.63	A
ATOM	293	0	GLY	A	38	55.369	-2.549	34.098	1.00 38.42	${f A}$
ATOM	294	N		A	39	54.101	-0.861	33.334	1.00 38.93	${f A}$
ATOM	295	CA		A	39	53.625	-0.499	34.660	1.00 40.81	A
					39	53.645	1.029	34.803	1.00 42.41	A
MOTA	296	CB	ARG	A.			1.627	34.339	1.00 44.76	A
ATOM	297	CG		A	39	54.968				
ATOM	298	CD	ARG	A	39	55.113	3.118	34.619	1.00 47.83	A
MOTA	299	NE	ARG	A	39	56.318	3.644	33.976	1.00 50.52	A
ATOM	300	CZ	ARG	A	39	56.902	4.799	34.281	1.00 53.40	A
ATOM	301	NHl	ARG	A	39	56.399	5.575	35.235	1.00 54.01	A
ATOM	302	NH2	ARG	A	39	57.998	5.179	33.633	1.00 54.18	Α
		C	ARG		39	52.229	-1.057	34.936	1.00 41.12	A
ATOM	303					51.664	-0.847	36.014	1.00 39.71	A
ATOM	304	0	ARG		39				1.00 40.65	A
MOTA	305	N	LYS		40	51.687	-1.779	33.955		
ATOM	306	CA	LYS	A	40	50.365	-2.380	34.070	1.00 39.55	A
MOTA	307	CB	LYS	A	40	50.415	-3.554	35.053	1.00 42.42	A
ATOM	308	CG	LYS	A	40	49.196	-4.467	34.996	1.00 46.46	A
ATOM	309	CD	LYS	A	40	49.266	-5.563	36.054	1.00 50.42	A
ATOM	310	CE	LYS		40	48.077	-6.513	35.947	1.00 51.25	A
		NZ			40	46.781	-5.779	35.970	1.00 52.15	A
MOTA	311					49.338	-1.348	34.540	1.00 37.45	A
ATOM	312	C	LYS		40				1.00 35.78	A
ATOM	313	0	LYS		40	48.647	-1.560	35.533		
MOTA	314	N	GLU	A	41	49.245	-0.237	33.812	1.00 35.81	A
ATOM	315	CA	GLU	A	41	48.317	0.847	34.142	1.00 33.83	A
ATOM	316	CB	GLU	A	41	49.077	2.079	34.655	1.00 36.46	A
ATOM	317	CG	GLU		41	49.660	1.997	36.049	1.00 41.33	A
ATOM	318	CD	GLU		41	50.500	3.224	36.374	1.00 44.23	A
		OE1			41	50.067	4.343	36.022	1.00 46.67	A
MOTA	319					51.585	3.076	36.981	1.00 45.55	А
MOTA	320	OE2			41			32.937	1.00 30.89	A
ATOM	321	C	GLU		41	47.492	1.301			
MOTA	322	0	GLU	Α	41	47.995	1.373	31.816	1.00 27.89	A
MOTA	323	N	THR	A	42	46.227	1.623	33.182	1.00 28.11	A
ATOM	324	CA	THR	. A	42	45.354	2.127	32.135	1.00 26.58	A
ATOM	325	CB	THR	. A	42	43.882	1.773	32.406	1.00 27.67	A
ATOM	326	OG1			42	43.716	0.349	32.394	1.00 25.55	A
	327	CG2			42	42.979	2.419	31.357	1.00 25.33	A
ATOM						45.506	3.642	32.212	1.00 26.90	A
MOTA	328	C	THR		42			33.269	1.00 25.79	A
ATOM	329	0	THR		42	45.305	4.232			
MOTA	330	N	VAL	A	43	45.881	4.273	31.108	1.00 25.87	A
ATOM	331	CA	VAL	A	43	46.045	5.720	31.106	1.00 24.36	A
ATOM	332	CB	VAL	A	43	47.474	6.119	30.670	1.00 24.45	A
ATOM	333	CG1	VAL	A	43	47.698	7.606	30.906	1.00 24.38	A
MOTA	334	CG2			43	48.504	5.289	31.433	1.00 22.82	A
			VAI		43	45.039	6.331	30.141	1.00 24.94	${f A}$
MOTA	335	C					6.133	28.930	1.00 24.72	A
MOTA	336	0	VAI		43	45.143			1.00 24.50	A
ATOM	337	N	TRE		44	44.063	7.065	30.672		
ATOM	338	$^{\mathrm{CA}}$	TRE	A	44	43.050	7.681	29.824	1.00 25.64	A
ATOM	339	CB	TRE	A	44	41.804	8.033	30.642	1.00 25.03	A
ATOM	340	CG	TRE	A	44	41.224	6.859	31.370	1.00 25.96	${f A}$
MOTA	341	CD2	TRE	A	44	40.281	5.906	30.858	1.00 25.77	A
ATOM	342	CE2			44	40.067	4.946	31.870	1.00 26.64	A
		CE3			44	39.599	5.766	29.641	1.00 24.94	A
ATOM	343				44	41.529	6.450	32.634	1.00 26.43	A
MOTA	344	CD1						32.942	1.00 26.28	A
MOTA	345	NEI			44	40.840	5.305			
MOTA	346	CZ2	TRI) A	44	39.197	3.860	31.704	1.00 25.00	A
MOTA	347	CZ3	TRI	? A	44	38.734	4.688	29.476	1.00 22.40	A
ATOM	348	CH2	TRI	? A	44	38.542	3.749	30.501	1.00 24.18	A
ATOM	349	C	TRI	P A	44	43.578	8.925	29.116	1.00 26.30	A
ATOM	350	0		? A	44	44.321	9.713	29.700	1.00 24.42	A
		N		5 A	45	43.193	9.090	27.853	1.00 28.01	A
MOTA	351					43.635		27.062	1.00 30.22	A
MOTA	352	CA		S A	45			25.666	1.00 29.51	A
MOTA	353	CB	CY		45	44.069				
MOTA	354	SG	CY			45.547		25.680	1.00 30.66	A
ATOM	355	C	CY	S A	45	42.574	11.317		1.00 31.06	A
ATOM	356	0	CY	S A	45	42.836	12.399	26.428	1.00 34.14	A
ATOM	357	N		A U		41.375	11.016	27.439	1.00 31.99	A
ATOM	358	CA		UΑ		40.261		27.436	1.00 32.61	A
		CB		U A		39.137		26.506	1.00 31.72	A
MOTA	359	CG		ÜΑ		38.810			1.00 32.47	A
ATOM	360									A
ATOM	361	CD:		U A		37.492				A
ATOM	362	CD:		U A		38.710			1.00 29.99	
ATOM	363	C		U A		39.734	_			A
MOTA	364	0	LE	U A	46	39.195	11.066		1.00 33.99	A
ATOM	365	N	PR	O A	47	39.893	13.201	29.521	1.00 32.52	A
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ATOM	366	CD	PRO	A	47	40.488	14.442	28.986	1.00 32.23	A
ATOM	367	CA	PRO	A	47	39.437	13.392	30.901	1.00 32.18	A
ATOM	368	CB	PRO	A	47	39.487	14.908	31.063	1.00 32.11	A
ATOM	369	CG	PRO	A	47	40.690	15.270	30.236	1.00 31.60	A
MOTA	370	C	PRO	Α	47	38.066	12.800	31.245	1.00 30.96	${f A}$
ATOM	371	0	PRO		47	37.927	12.103	32.243	1.00 30.17	A
			VAL		48	37.064	13.068	30.418	1.00 30.75	A
ATOM	372	N								A
ATOM	373	CA	VAL		48	35.715	12.563	30.663		
ATOM	374	CB	VAL		48	34.748	13.040	29.560	1.00 34.04	A
MOTA	375	CG1	VAL	A	48	33.320	12.683	29.932	1.00 34.16	A
MOTA	376	CG2	VAL	A	48	34.881	14.556	29.368	1.00 38.02	A
ATOM	377	C	VAL	A	48	35.633	11.033	30.765	1.00 33.13	\mathbf{A}
ATOM	378	0	VAL	A	48	34.698	10.485	31.355	1.00 33.55	A
ATOM	379	N	LEU	A	49	36.615	10.350	30.192	1.00 33.30	A
ATOM	380	CA	LEU		49	36.661	8.892	30.208	1.00 32.44	A
ATOM	381	CB	LEU	A	49	37.498	8.391	29.023	1.00 30.62	A
			LEU		49	36.792	8.027	27.702	1.00 31.64	A
ATOM	382	CG							1.00 32.04	A
	383	CD1	LEU	A	49	35.578	8.888	27.464		
ATOM	384	CD2	LEU		49	37.783	8.157	26.551	1.00 31.05	A
MOTA	385	С	LEU	A	49	37.226	8.343	31.519	1.00 33.77	A
MOTA	386	0	LEU	A	49	37.138	7.142	31.787	1.00 34.14	A
ATOM	387	N	ARG	A	50	37.794	9.221	32.339	1.00 34.56	A
ATOM	388	CA	ARG	A	50	38.367	8.810	33.618	1.00 35.58	A
ATOM	389	CB	ARG	A	50	38.987	10.009	34.345	1.00 37.99	A
ATOM	390	CG	ARG		50	40.137	10.720	33.636	1.00 40.65	A
MOTA	391	CD	ARG		50	40.657	11.846	34.529	1.00 43.05	A
		NE	ARG		50	41.603	12.748	33.872	1.00 44.85	A
ATOM	392						12.403	33.444	1.00 46.08	A
ATOM	393	CZ	ARG		50	42.815				
ATOM	394	NHl	ARG		50	43.254	11.159	33.592	1.00 46.76	A
ATOM	395	NH2	ARG	A	50	43.599	13.314	32.880	1.00 46.08	A
ATOM	396	C	ARG	A	50	37.334	8.168	34.547	1.00 35.55	A
MOTA	397	0	ARG	A	50	37.693	7.475	35.495	1.00 35.21	A
ATOM	398	N	GLN	A	51	36.054	8.412	34.284	1.00 36.77	A
ATOM	399	CA	GLN	A	51	34.987	7.859	35.116	1.00 37.34	A
ATOM	400	СВ	GLN		51	33.658	8.558	34.821	1.00 39.02	A
ATOM	401	CG	GLN		51	33.123	8.306	33.418	1.00 41.24	A
		CD	GLN		51	31.765	8.947	33.189	1.00 43.49	A
ATOM	402					30.781	8.597	33.843	1.00 43.80	A
ATOM	403	OE1	GLN		51				1.00 44.01	A
MOTA	404	NE2	GLN		51	31.706	9.895	32.260		
ATOM	405	C	GLN		51	34.821	6.362	34.896	1.00 36.85	A
MOTA	406	0	GLN	A	51	34.250	5.665	35.734	1.00 37.06	A
MOTA	407	N	PHE	A	52	35.316	5.871	33.764	1.00 35.13	A
MOTA	408	CA	PHE	A	52	35.218	4.454	33.446	1.00 32.82	A
MOTA	409	CB	PHE	A	52	35.143	4.258	31.931	1.00 31.28	A
ATOM	410	CG	PHE	A	52	33.902	4.838	31.301	1.00 29.86	A
ATOM	411	CD1			52	32.640	4.549	31.821	1.00 27.82	A
MOTA	412	CD2			52	33.992	5.652	30.177	1.00 27.71	A
		CE1			52	31.490	5.060	31.234	1.00 25.58	A
ATOM	413						6.171	29.580	1.00 28.10	A
ATOM	414	CE2			52	32.847				
ATOM	415	CZ	PHE		52	31.592	5.873	30.111	1.00 28.21	A
MOTA	416	C	PHE	A	52	36.405	3.675	34.004	1.00 32.57	A
ATOM	417	0	PHE	A	52	37.370	4.256	34.494	1.00 32.22	A
ATOM	418	N	ARG	A	53	36.327	2.353	33.927	1.00 32.80	A
MOTA	419	CA	ARG	A	53	37.397	1.498	34.419	1.00 32.77	A
ATOM	420	CB	ARG	A	53	37.005	0.862	35.760	1.00 36.56	A
ATOM	421	CG	ARG	A	53	36.741	1.867	36.881	1.00 42.83	A
ATOM	422	CD	ARG	A	53	36.523	1.168	38.214	1.00 49.04	A
ATOM	423	NE	ARG		53	36.308	2.111	39.312	1.00 53.82	A
	424	CZ	ARG		53	36.195	1.758	40.589	1.00 54.70	A
ATOM						36.277	0.478	40.937	1.00 55.50	A
MOTA	425	NH1			53				1.00 55.64	
MOTA	426	NH2			53	36.004	2.683	41.520		A
MOTA	427	C	ARG		53	37.706	0.404	33.405	1.00 29.88	A
MOTA	428	0	ARG	A	53	36.806	-0.117	32.743	1.00 28.71	A
ATOM	429	N	PHE	A	54	38.986	0.066	33.293	1.00 26.44	A
ATOM	430	CA	PHE	A	54	39.440	-0.960	32.371	1.00 22.47	A
ATOM	431	CB	PHE	A	54	39.905	-0.325	31.060	1.00 21.88	A
ATOM	432	CG	PHE		54	40.181	-1.320	29.974	1.00 20.69	A
ATOM	433	CD1			54	39.150	-1.801	29.180	1.00 19.52	A
ATOM	434		PHE		5 4 54	41.471	-1.782	29.750	1.00 18.68	A
	435		. PHE		5 4	39.399	-2.734	28.170	1.00 22.81	A
MOTA						41.733	-2.734	28.746	1.00 20.58	A
ATOM	436	CE2			54 54			27.954	1.00 20.86	A
MOTA	437	CZ	PHE		54	40.697	-3.190			
MOTA	438	C	PHE		54	40.597	-1.711	33.017	1.00 23.43	A
MOTA	439	0	PHE	A	54	41.631	-1.122	33.351	1.00 23.53	A

ATOM	440	N	ASP	A	55	40.408	-3.011	33.198	1.00 22.82	A
ATOM	441	CA	ASP	A	55	41.411	-3.874	33.805	1.00 24.70	A
ATOM	442	CB	ASP	A	55	40.785	-5.246	34.083	1.00 23.26	A
ATOM	443	CG	ASP	A	55	41.729	-6.190	34.789	1.00 26.24	A
MOTA	444	OD1	ASP	A	55	42.924	-5.853	34.933	1.00 28.75	A
ATOM	445	OD2	ASP	A	55	41.274	-7.279	35.192	1.00 26.38	A
ATOM	446	C	ASP	A	55	42.613	-4.011	32.861	1.00 24.24	A
ATOM	447	0	ASP	A	55	42.510	-4.629	31.802	1.00 23.91	A
MOTA	448	N	PRO	A	56	43.770	-3.437	33.238	1.00 23.69	A
ATOM	449	CD	PRO	A	56	44.084	-2.761	34.509	1.00 23.79	A
ATOM	450	CA	PRO		56	44.961	-3.522	32.387	1,00 23.45	A
ATOM	451	CB	PRO		56	46.002	-2.707	33.162	1.00 23.35	A
ATOM	452	CG	PRO		56	45.592	-2.897	34.580	1.00 23.31	A
MOTA	453	C	PRO		56	45.413	-4.952	32.114	1.00 23.66	A
MOTA	454	0	PRO		56	46.099	-5.220	31.125	1.00 23.15	A
ATOM	455	N	GLN		57	45.025	-5.871	32.991	1.00 21.84	A
ATOM	456	CA	GLN		57	45.397	-7.261	32.818	1.00 22.47 1.00 23.11	A A
ATOM	457	CB	GLN		57	44.834	-8.108	33.965	1.00 23.11 1.00 20.82	A
ATOM	458	CG	GLN		57	45.226	-9.568 -9.745	33.873 33.733	1.00 20.82	A
ATOM	459	CD	GLN		57 57	46.722 47.497	-9.745 -9.227	34.539	1.00 22.23	A
ATOM	460	OE1 NE2	GLN GLN		57 57	47.138	-10.475	32.707	1.00 23.15	A
ATOM	461 462	C NF2	GLN		5 <i>7</i>	44.882	-7.792	31.482	1.00 22.21	A
ATOM ATOM	462	0	GLN		57	45.452	-8.723	30.913	1.00 23.00	A
ATOM	463	И	PHE		58	43.801	-7.203	30.980	1.00 22.42	A
ATOM	465	CA	PHE		58	43.254	-7.640	29.704	1.00 21.07	A
ATOM	466	CB	PHE		58	42.004	-6.857	29.338	1.00 20.45	A
ATOM	467	CG	PHE		58	41.411	-7.287	28.031	1.00 21.03	A
ATOM	468	CD1	PHE		58	40.472	-8.312	27.988	1.00 18.42	A
MOTA	469		PHE		58	41.864	-6.736	26.835	1.00 18.79	A
ATOM	470	CE1	PHE		58	39.992	-8.792	26.765	1.00 21.25	A
ATOM	471	CE2	PHE	A	58	41.393	-7.207	25.610	1.00 20.28	A
ATOM	472	CZ	PHE	A	58	40.457	-8.238	25.578	1.00 21.18	A
ATOM	473	C	PHE	A	58	44.278	-7.401	28.612	1.00 21.79	Α
ATOM	474	0	PHE	A	58	44.529	-8.260	27.763	1.00 21.84	A
ATOM	475	N	ALA	A	59	44.849	-6.202	28.637	1.00 21.80	A
MOTA	476	CA	ALA	A	59	45.840	-5.801	27.657	1.00 21.67	A
ATOM	477	CB	ALA	A	59	46.254	-4.346	27.892	1.00 21.11	A
ATOM	478	C	ALA	A	59	47.053	-6.711	27.732	1.00 22.06	A
ATOM	479	0	ALA	A	59	47.518	-7.213	26.706	1.00 22.53	A
ATOM	480	N	LEU	A	60	47.561	-6.925	28.945	1.00 19.83	A
MOTA	481	CA	LEU	A	60	48.729	-7.777	29.116	1.00 20.88	A
MOTA	482	CB	LEU		60	49.163	-7.815	30.585	1.00 20.57	A
MOTA	483	CG	LEU		60	50.060	-6.657	31.053	1.00 24.17	A
ATOM	484	CD1			60	49.239	-5.392	31.205	1.00 24.16	A
ATOM	485	CD2			60	50.717	-7.012	32.382	1.00 24.31	A
MOTA	486	C	LEU		60	48.496	-9.193	28.598	1.00 20.44	A
ATOM	487	0	LEU		60	49.367	-9.770	27.955	1.00 21.97	A
ATOM	488	N	THR		61	47.319	-9.749	28.871 28.418	1.00 20.69 1.00 19.49	A A
ATOM	489	CA	THR		61		-11.101 -11.629	29.084	1.00 19.49	A
ATOM	490	CB	THR		61		-11.830	30.489	1.00 13.33	A
ATOM	491	OG1 CG2			61 61		-12.942	28.453	1.00 21.12	A
ATOM	492 493	CGZ	THR		61		-11.140	26.903	1.00 19.22	A
MOTA ATOM	494	0	THR		61		-12.059	26.242	1.00 21.19	Ą
ATOM	495	N	ASN		62		-10.142	26.351	1.00 18.05	A
ATOM	496	CA	ASN		62		-10.092	24.910	1.00 19.26	A
ATOM	497	CB	ASN		62	45.020		24.552	1.00 20.51	A
ATOM	498	CG	ASN		62	43.835		23.680	1.00 22.06	A
ATOM	499	OD1			62	43.406		23.693	1.00 21.71	A
ATOM	500	ND2			62	43.294	-8.371	22.930	1.00 20.64	A
ATOM	501	C	ASN		62	47.270	-9.975	24.188	1.00 18.14	A
ATOM	502	0	ASN		62	47.517	-10.681	23.217	1.00 19.73	A
MOTA	503	N	ILE		63	48.146	-9.108	24.684	1.00 18.98	A
ATOM	504	CA	${ m ILE}$	A	63	49.448	-8.921	24.061	1.00 19.88	A
ATOM	505	CB	ILE	Α	63	50.229	-7.757	24.725	1.00 21.31	A
ATOM	506	CG2	ILE	A	63	51.601	-7.590	24.064	1.00 20.11	A
MOTA	507	CG1	. ILE	A	63	49.425	-6.457	24.599	1.00 20.91	A
MOTA	508	CD1	. ILE	A	63	49.037	-6.092	23.171	1.00 16.67	A
ATOM	509	C	ILE	Α	63,	50.247		24.169	1.00 20.35	A
MOTA	510	0	ILE	A	63		-10.538	23.297	1.00 21.37	A
MOTA	511	N	ALA		64	50.028		25.247	1.00 22.48	A
MOTA	512	CA	ALA		64	50.713		25.423	1.00 23.35	A
MOTA	513	CB	ALA	A	64	50.373	-12.816	26.785	1.00 22.29	A

MOTA	514	С	ALA A	64	50.252	-13.158	24.301	1.00 23.03	A
ATOM	515	0	ALA A	64	51.032	-13.939	23.766	1.00 25.08	A
ATOM	516	N	VAL A	65	48.976	-13.072	23.948	1.00 23.28	A
ATOM		CA	VAL A	65	48.437	-13.905	22.888	1.00 22.97	A
	517				46.887	-13.840	22.859	1.00 24.28	A
MOTA	518	CB	VAL A	65					
ATOM	519	CG1	VAL A	65	46.338	-14.722	21.729	1.00 22.40	A
MOTA	520	CG2	VAL A	65	46.325	-14.296	24.209	1.00 19.61	A
MOTA	521	C	VAL A	65	49.013	-13.471	21.538	1.00 23.88	A
ATOM	522	0	VAL A	65	49.313	-14.314	20.692	1.00 22.01	A
ATOM	523	N	LEU A	66	49.179	-12.164	21.332	1.00 24.00	A
ATOM	524	CA	LEU A	66	49.747	-11.692	20.064	1.00 24.66	A
						-10.171	20.011	1.00 22.13	A
MOTA	525	CB	LEU A	66	49.872				
ATOM	526	CG	LEU A	66	48.679	-9.228	20.117	1.00 23.81	A
MOTA	527	CD1	LEU A	66	49.014	-8.001	19.277	1.00 20.24	A
MOTA	528	CD2	LEU A	66	47.407	-9.866	19.627	1.00 20.49	A
ATOM	529	C	LEU A	66	51.143	-12.267	19.906	1.00 23.53	A
ATOM	530	0	LEU A	66	51.548	-12.644	18.813	1.00 22.08	A
ATOM	531	N	LYS A	67	51.879	-12.303	21.011	1.00 26.17	A
ATOM		CA	LYS A	67	53.237	-12.832	21.019	1.00 28.99	A
	532				53.839	-12.698	22.421	1.00 29.27	A
MOTA	533	CB	LYS A	67					
ATOM	534	CG	LYS A	67	55.278	-13.174	22.548		A.
MOTA	535	CD	LYS A	67	55.779	-13.001	23.976	1.00 32.41	A
ATOM -	536	CE	LYS A	67	57.159	-13.609	24.157	1.00 35.25	A
MOTA	537	NZ	LYS A	67	58.144	-13.036	23.199	1.00 38.78	A
ATOM	538	C	LYS A	67	53.200	-14.299	20.598	1.00 29.87	A
ATOM	539	0	LYS A	67	53.952	-14.719	19.716	1.00 30.35	A
		N	HIS A	68	52.313	-15.066	21.230	1.00 30.48	A
MOTA	540				52.163	-16.483	20.922	1.00 31.95	A
MOTA	541	CA	HIS A	68					
ATOM	542	CB	HIS A	68	51.051		21.775	1.00 34.42	A
ATOM	543	CG	HIS A	68	50.827	-18.557	21.520	1.00 38.63	A
ATOM	544	CD2	HIS A	68	, 49.859	-19.203	20.826	1.00 40.18	A
ATOM	545	ND1	HIS A	68	51.676	-19.536	21.992	1.00 41.00	A
ATOM	546	CE1	HIS A	68	51.241	-20.721	21.601	1.00 39.93	A
ATOM	547	NE2		68	50.141	-20.547	20.891	1.00 39.69	A
		C	HIS A	68	51.828		19.448	1.00 31.53	A
ATOM	548						18.746	1.00 32.07	A
MOTA	549	0	HIS A	68	52.463				
ATOM	550	N	ASN A	69	50.826		18.977	1.00 29.53	A
ATOM	551	CA	ASN A	69	50.427	-16.024	17.583	1.00 29.99	A
MOTA	552	CB	ASN A	69	49.180	-15.173	17.332	1.00 30.27	A
ATOM	553	CG	ASN A	69	47.918	-15.814	17.885	1.00 31.83	A
ATOM	554	OD1		69	47.986	-16.728	18.703	1.00 32.19	A
		ND2		69	46.759		17.447	1.00 31.41	A
ATOM	555						16.638	1.00 30.37	A
ATOM	556	C	ASN A	69	51.552				
ATOM	557	0	ASN A	69	51.722		15.571	1.00 29.41	A
MOTA	558	N	LEU A	70	52.324	-14.593	17.026	1.00 29.86	A
ATOM	559	CA	LEU A	70	53.413	-14.131	16.175	1.00 31.35	A
ATOM	560	CB	LEU A	70	54.039	-12.857	16.751	1.00 28.55	A
ATOM	561	CG	LEU A	70	55.190	-12.237	15.950	1.00 28.77	A
ATOM	562	CD1		70	54.745	-11.949	14.519	1.00 28.48	A
ATOM	563	CD2		70	55.651		16.627	1.00 27.89	A
						-15.214	16.009	1.00 31.92	A
MOTA	564	C	LEU A	70			14.914	1.00 31.72	A
ATOM	565	0	LEU A	70		-15.422			
MOTA	566	N	asn a	71		-15.905	17.097	1.00 34.09	A
MOTA	567	ÇA	ASN A	71		-16.968	17.060	1.00 38.27	A
MOTA	568	CB	ASN A	71	55.884	-17.651	18.427	1.00 39.70	A
ATOM	569	CG	ASN A	71	56.490	-16.748	19.490	1.00 44.05	${f A}$
ATOM	570	OD1	ASN A	71	56.290	-16.955	20.693	1.00 44.98	A
ATOM	571	ND2		71		-15.746	19.049	1.00 44.44	A
		C				-18.003	15.983	1.00 38.32	A
ATOM	572		ASN A				15.224	1.00 37.91	. A
MOTA	573	0	ASN A	71		-18.417			
ATOM	574	N	SER A			18.407	15.919	1.00 39.49	A
MOTA	575	CA	SER A	72	· ·	-19.390	14.944	1.00 40.10	A
ATOM	576	CB	SER A	72	52.341	-19.816	15.256	1.00 41.05	A
MOTA	577	OG	SER A	72	51.867	-20.763	14.311	1.00 42.44	A
ATOM	578	C	SER A			-18.838	13.523	1.00 40.66	A
ATOM	579	0	SER A			-19.516	12.608	1.00 40.90	A
						-17.608	13.341	1.00 39.86	A
ATOM	580	N	LEU A					1.00 39.32	A
ATOM	581	CA	LEU A			-16.973	12.030		
ATOM	582	CB	LEU A			-15.632	12.082	1.00 38.99	A
MOTA	583	CG	LEU A	73		-15.651	11.598	1.00 40.31	A
MOTA	584	CD:	L LEU A	73	50.482	2 -16.860	12.152	1.00 39.79	A
ATOM	585	CD:	LEU A	73	50.539	-14.363	12.024	1.00 40.04	A
ATOM	586	C	LEU A			-16.778	11.492	1.00 38.55	A
	587	0	LEU A			3 -16.806	10.280	1.00 36.83	A
ATOM	J 4 7	•	Line Pr	. , ,	55.020				- -

ATOM	588	N	ILE A	74	55.780 -1		12.383 11.942	1.00 39.70 1.00 41.87	A A
ATOM ATOM	589 590	CA CB	ILE A	74 74		L6.402 L6.084	13.123	1.00 41.88	A
ATOM ATOM	590 591	CG2	ILE A	74		L6.054	12.640	1.00 41.29	A
ATOM	592	CG1	ILE A	74	57.729 - 3	L4.734	13.738	1.00 41.53	A
ATOM	593	CD1	ILE A	74		L4.380	14.990	1.00 40.94	A
MOTA	594	C	ILE A	74		17.699	11.273	1.00 42.04	A.
ATOM	595	0	ILE A	74 75	58.119 -: 57.364 -:	17.689 18.816	10.157 11.954	1.00 41.12 1.00 43.51	A A
ATOM ATOM	596 597	N CA	LYS A	75 75		20.125	11.423	1.00 46.61	A
ATOM	597 598	CB	LYS A	75 75		21.217	12.466	1.00 47.84	A
ATOM	599	CG	LYS A		58.096 -2	20.964	13.828	1.00 50.82	A
ATOM	600	CD	LYS A	75		22.029	14.828	1.00 53.97	A
ATOM	601	CE	LYS A		58.005 -		16.269	1.00 55.95	· A A
ATOM	602	NZ	LYS A		59.472 -: 56.944 -:	21.572 20.452	16.531 10.151	1.00 56.31 1.00 47.99	A
ATOM ATOM	603 604	С О	LYS A		57.530 -		9.106	1.00 48.11	A
ATOM	605	И	ARG A			20.419	10.242	1.00 49.31	A
ATOM	606	CA	ARG A		54.763 -	20.742	9.103	1.00 50.89	A
ATOM	607	CB	ARG A	76	 	20.744	9.530	1.00 53.08	A
MOTA	608	CG	ARG A		-	21.847	10.538	1.00 56.83	A
ATOM	609	CD	ARG A	_	51.478 -: 50.620 -:	22.247	10.574 11.212	1.00 58.85 1.00 60.24	A A
MOTA MOTA	610 611	NE CZ	ARG A		49.786		10.557	1.00 61.29	A
ATOM	612		ARG A		49.692 -		9.234	1.00 60.08	A
ATOM	613	NH2			49.044 -	19.578	11.226	1.00 61.97	A
ATOM	614	C	ARG A	. 76	54.947 -		7.864	1.00 50.93	A
MOTA	615	0	ARG A		54.705 -		6.747	1.00 51.19 1.00 50.61	A A
ATOM	616	N	SER A		55.380 - 55.574 -		8.046 6.900	1.00 50.01	A
ATOM ATOM	617 618	CA CB	SER A		55.262 -		7.282	1.00 50.05	A
ATOM	619	OG	SER A			15.787	8.193	1.00 49.23	A
ATOM	620	C	SER A		57.006 -	17.827	6.386	1.00 49.56	A
ATOM	621	0	SER A	. 77	- · · · · · · · · · · · · · · · · · · ·	17.015	5.558	1.00 49.40	A
MOTA	622	N	ASN A			18.817	6.866	1.00 49.24 1.00 49.14	A A
ATOM	623	CA	ASN A		59.148 - 59.256 -	18.982	6.472 4.976	1.00 49.14	A
ATOM ATOM	624 625	CB CG	ASN A		60.668 -		4.558	1.00 48.09	A
ATOM	626	OD1			61.347 -		5.254	1.00 46.05	A
ATOM	627	ND2		78	61.109 -	19.182	3.409	1.00 47.78	A
MOTA	628	C	ASN A		59.857 -		6.803	1.00 49.08	A
ATOM	629	0	ASN A		60.614 - 59.571 -		6.001 8.006	1.00 48.39 1.00 48.58	A A
MOTA	630	N CA	SER A		60.139 -		8.538	1.00 48.38	A
ATOM ATOM	631 632	CB	SER A			16.208	9.071	1.00 48.53	A
ATOM	633	OG	SER A		62.415 -	16.612	8.027	1.00 50.05	A
ATOM	634	C	SER A	A 79	60.176 -		7.573	1.00 47.13	A
MOTA	635	0	SER A		• •	14.098	7.444	1.00 47.66 1.00 45.82	A A
ATOM	636	N	THR A		59.069 - 59.008 -	14.516	6.887 5.982	1.00 45.82	A
ATOM ATOM	637 638	CA CB	THR A		57.814 -		5.016	1.00 47.03	A
ATOM	639	OG1				-13.963	5.731	1.00 47.95	A
ATOM	640	CG2		08 <i>I</i>	58.134 -	14.487	3.909	1.00 47.59	A
ATOM	641	C	THR A			-12.147	6.882	1.00 44.25	A.
ATOM	642	0	THR A			-11.976 -11.311	7.556 6.903	1.00 43.69 1.00 41.47	A A
ATOM ATOM	643 644	N CA	ALA A		·	-10.119	7.740	1.00 38.59	A
ATOM	645	CB	ALA A		61.363	-9.734	8.039	1.00 38.61	A
ATOM	646	C	ALA A		59.168	-8.915	7.185	1.00 36.89	A
MOTA	647	0	ALA A	A 81	58.766	-8.884	6.018	1.00 35.83	A
MOTA	648	N	ALA A		58.993	-7.920	8.050	1.00 34.86 1.00 33.41	A A
ATOM	649	CA	ALA A		58.300 57.957	-6.690 -5.912	7.698 8.961	1.00 33.41	A
ATOM ATOM	650 651	CB C	ALA A		59.141	-5.824	6.770	1.00 32.28	A
ATOM	652		ALA I		60.372	-5.807	6.859	1.00 28.62	A
ATOM	653	N	THR		58.457	-5.113	5.878	1.00 31.60	A
MOTA	654	CA	THR I	A 83	59.100	-4.217	4.931	1.00 32.87	A
ATOM	655		THR I		58.377	-4.224	3.575	1.00 34.31 1.00 36.90	A A
ATOM	656 657				58.347 59.098	-5.562 -3.309	3.058 2.578	1.00 36.90	A
ATOM ATOM	657 658		2 THR 2 THR 2		59.098	-2.808	5.500	1.00 32.84	A
MOTA	659		THR .		58.029	-2.406	6.067	1.00 33.97	A
MOTA	660		ASN .		60.130	-2.062	5.356	1.00 34.76	A
MOTA	661	CA	ASN .	A 84	60.188	-0.697	5.858	1.00 34.66	A

ATOM	662	СВ	ASN	A	84	61.634	-0.252	6.069	1.00 36.13	A
ATOM	663	CG	ASN	A	84	62.337	-1.045	7.132	1.00 37.22	A
ATOM	664		ASN		84	61.809	-1.241	8.220	1.00 39.34	A
ATOM	665		ASN		84	63.548	-1.497	6.830	1.00 38.89	A
ATOM	666	C	ASN		84	59.549	0.267	4.881	1.00 35.51	A
ATOM	667	0	ASN		84	59.961	0.343	3.724	1.00 38.89	A
ATOM	668	N	GLU		85	58.546	1.004	5.344	1.00 34.17	A
ATOM	669	CA	GLU		85	57.890	2.001	4.507	1.00 32.82	A
ATOM	670	CB	GLU		85	56.427	2.183	4.921	1.00 36.55	A
		CG	GLU		85	55.523	0.993	4.645	1.00 42.74	A
MOTA	671		GLU		85	55.271	0.782	3.167	1.00 46.65	A
ATOM	672	CD			85	54.829	1.741	2.494	1.00 49.22	A
ATOM	673	OE1	GLU			55.508	-0.345	2.679	1.00 48.74	A
ATOM	674	OE2	GLU		85			4.701	1.00 30.10	A
ATOM	675	C	GLU		85	58.624	3.328	5.571	1.00 30.10	A
MOTA	676	0	GLU		85	59.489	3.453	3.878	1.00 27.23	A
ATOM	677	N	JAV		86	58.274	4.308		1.00 23.37	A
ATOM	678	CA	VAL		86	58.849	5.641	3.951	1.00 27.33	A
ATOM	679	CB	VAL		86	59.146	6.202	2.539		
ATOM	680	CG1	VAL		86	59.688	7.637	2.640	1.00 22.06	A.
ATOM	681	CG2	VAL		86	60.139	5.289	1.815	1.00 25.30	A
MOTA	682	С	VAL	A	86	57.786	6.519	4.614	1.00 27.98	A
MOTA	683	0	LAV	A	86	56.685	6.671	4.086	1.00 28.76	A ~
MOTA	684	N	PRO	A	87	58.095	7.098	5.784	1.00 27.39	A
ATOM	685	CD	PRO	A	87	59.268	6.861	6.644	1.00 26.00	A
MOTA	686	CA	PRO	A	87	57.106	7.949	6.458	1.00 28.38	A
ATOM	687	CB	PRO	A	87	57.611	7.989	7.899	1.00 26.97	A
MOTA	688	CG	PRO	A	87	59.099	7.915	7.727	1.00 27.97	A
ATOM	689	С	PRO	A	87	56.963	9.341	5.848	1.00 30.15	A
ATOM	690	0	PRO	A	87	57.902	9.871	5.245	1.00 31.62	A
ATOM	691	N	GLU	A	88	55.778	9.922	6.004	1.00 29.70	A
ATOM	692	CA	GLU		88	55.489	11.252	5.481	1.00 29.65	A
ATOM	693	CB	GLU		88	54.173	11.229	4.699	1.00 32.09	A
ATOM	694	CG	GLU		88	54.038	12.330	3.655	1.00 38.40	A
ATOM	695	CD	GLU		88	52.790	12.172	2.792	1.00 41.07	A
ATOM	696	OE1			88	51.675	12.411	3.303	1.00 42.35	A
		OE2			88	52.925	11.800	1.604	1.00 43.46	A
ATOM	697		GLU		88	55.385	12.191	6.680	1.00 27.98	A
ATOM	698	C			88	54.588	11.954	7.597	1.00 26.16	A
MOTA	699	0	GLU			56.187	13.253	6.672	1.00 23.90	A
ATOM	700	N	VAL		89		14.194	7.788	1.00 21.62	A
MOTA	701	CA	VAL		89	56.201		8.333	1.00 21.02	A
MOTA	702	CB	VAL		89	57.637	14.358		1.00 13.30	A
MOTA	703	CG1			89	57.639	15.295	9.534		A
ATOM	704	CG2			89	58.204	12.990	8.719	1.00 16.77	
ATOM	705	C	VAL		89	55.626	15.575	7.483	1.00 21.60	A
MOTA	706	0	VAL		89	55.859	16.143	6.420	1.00 21.72	A
MOTA	707	N	THR	A	90	54.886	16.115	8.444	1.00 21.28	A
MOTA	708	CA	THR	A	90	54.269	17.425	8.301	1.00 20.62	A
MOTA	709	CB	THR	A	90	52.813	17.303	7.823	1.00 21.90	A
ATOM	710	OG1	THR	A	90	52.770	16.537	6.613	1.00 26.43	A
ATOM	711	CG2	THR	L A	90	52.220	18.678	7.558	1.00 23.70	A
MOTA	712	C	THR	A	90	54.264	18.153	9.639	1.00 21.08	A
ATOM	713	0	THE	A J	90	53.887	17.578	10.667	1.00 20.41	A
ATOM	714	N	VAI	A	91	54.670	19.423	9.618	1.00 19.24	A
MOTA	715	CA	VAI	A	91	54.712	20.243	10.822	1.00 19.55	A
MOTA	716	CB	IAV	A	91	56.149	20.739	11.102	1.00 19.97	A
ATOM	717	CG1	. VAI	A	91	56.167	21.629	12.338	1.00 16.82	A
MOTA	718	CG2	XAI	A	91	57.072	19.547	11.280	1.00 17.43	A
ATOM	719	C	VAI		91	53.789	21.452	10.703	1.00 19.10	A
ATOM	720	0	VAI		91	53.735	22.108	9.666	1.00 20.59	A
ATOM	721	N	PHE		92	53.059	21.739	11.772	1.00 18.65	A
ATOM	722	CA		A	92	52.146	22.870	11.785	1.00 19.10	A
ATOM	723	CB		A	92	50.853	22.516	11.030	1.00 18.89	A
ATOM	724	CG	PHE		92	50.176	21.264	11.525	1.00 16.16	A
ATOM	725	CD1			92	49.165	21.331	12.480	1.00 16.77	A
ATOM	725	CD2				50.561	20.017	11.047	1.00 16.62	A
		CE1		E A		48.543	20.168	12.955	1.00 18.06	A
MOTA	727					49.954	18.848	11.511	1.00 18.17	A
ATOM	728	CE2		E A	92	48.936	18.922	12.471	1.00 17.05	A
MOTA	729	CZ	PHI		92	51.844	23.236	13.229	1.00 17.05	A
ATOM	730	C		EA		51.844		14.134	1.00 19.48	A
ATOM	731	0		EA				13.445	1.00 19.64	A
ATOM	732			R A		51.365			1.00 18.69	A
MOTA	733	CA		R A		51.052		14.792		A
MOTA	734			R A		51.275		14.921	1.00 17.24	A
MOTA	735	OG	SE	R A	93	50.435	27.132	14.043	1.00 20.17	A
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ATOM	736	C	SER	A	93	49.618	24.554	15.172	1.00 19.04	A
ATOM	737	0	SER		93	48.748	24.417	14.316	1.00 17.44	A
ATOM	738		•	A	94	49.390	24.418	16.472	1.00 20.26	A
ATOM	739			A	94	48.077	24.108	17.010 18.464	1.00 21.70 1.00 22.45	A A
ATOM ATOM	740 741			A A	94 94	48.227 46.938	23.670 23.273	19.139	1.00 22.45	A
ATOM	742			A	94	47.189	22.867	20.587	1.00 25.48	A
ATOM	743	CE		A	94	45.881	22.548	21.297	1.00 25.73	A
ATOM	744	NZ	LYS		94	45.122	21.533	20.517	1.00 26.34	A
ATOM	745	C		A	94	47.169	25.340	16.921	1.00 23.44	A
ATOM	746	0	LYS	A	94	45.984	25.235	16.598	1.00 20.95	A
MOTA	747	N	SER	A	95	47.742	26.505	17.212	1.00 24.82	A
ATOM	748	CA	SER		95	47.013	27.769	17.172	1.00 27.69	A
ATOM	749	CB	SER		95	46.969	28.408	18.565	1.00 26.33	A
ATOM	750	OG	SER		95 05	46.202 47.688	27.635 28.747	19.468 16.219	1.00 32.56 1.00 27.36	A A
ATOM ATOM	751 752	С О	SER SER		95 95	48.824	28.747	15.797	1.00 27.94	A
ATOM	753	И	PRO		96	46.985	29.830	15.849	1.00 27.27	A
ATOM	754	CD	PRO		96	45.611	30.232	16.193	1.00 28.85	A
ATOM	755	CA	PRO	A	96	47.606	30.801	14.946	1.00 26.90	A
ATOM	756	CB	PRO	A	96	46.471	31.788	14.663	1.00 28.13	A
ATOM	757	CG	PRO	A	96	45.634	31.719	15.907	1.00 28.36	A
MOTA	758	C		A	96	48.786	31.421	15.700	1.00 24.92	A
ATOM	759	0		A	96	48.757	31.556	16.925	1.00 24.65	A
ATOM	760	N	VAL		97 97	49.828 51.016	31.786 32.332	14.973 15.601	1.00 24.24 1.00 25.15	A A
MOTA	761 762	CA CB	VAL VAL		97 97	52.261	32.332	14.715	1.00 26.78	A
ATOM ATOM	763	CG1	VAL		97	53.531	32.372	15.508	1.00 26.15	A
ATOM	764		VAL		97	52.255	30.659	14.198	1.00 26.15	A
ATOM	765	C	VAL		97	50.935	33.820	15.920	1.00 25.62	A
ATOM	766	0	VAL	A	97	50.624	34.638	15.054	1.00 25.01	A
ATOM	767	N	THR	A	98	51.207	34.157	17.175	1.00 24.46	A
MOTA	768	CA	THR		98	51.212	35.542	17.627	1.00 25.36	A
ATOM	769	CB	THR		98	49.835	35.941	18.283	1.00 25.29	A
ATOM	770	OG1	THR		98	50.030	37.008	19.217 18.985	1.00 30.50 1.00 29.80	A A
ATOM	771	CG2	THR		98 98	49.196 52.382	34.771 35.678	18.605	1.00 24.87	A
ATOM ATOM	772 773	C O	THR		98	52.382	34.902	19.554	1.00 23.01	A
ATOM	774	N	LEU		99	53.273	36.634	18.344	1.00 25.94	A
ATOM	775	CA	LEU		99	54.445	36.843	19.198	1.00 28.02	A
ATOM	776	CB	LEU		99	55.194	38.114	18.797	1.00 31.12	A
ATOM	777	CG	LEU	A	99	55.950	38.211	17.469	1.00 35.44	A
ATOM	778	CD1	LEU	A	99	56.650	39.577	17.416	1.00 35.45	A
MOTA	779	CD2	LEU		99	56.970	37.087	17.341	1.00 35.62	A
ATOM	780	C	LEU		99	54.135	36.932 37.616	20.689 21.097	1.00 27.10 1.00 25.34	A A
ATOM	781	O N	GLY		99	53.201 54.935	36.233	21.492	1.00 25.34	A
ATOM ATOM	782 783	N CA	GLY			54.762	36.253	22.935	1.00 26.48	A
ATOM	784	C	GLY			53.635	35.398	23.479	1.00 26.32	A
ATOM	785	0	GLY			53.428	35.323	24.695	1.00 25.37	A
ATOM	786	N	GLN	A	101	52.913	34.734	22.585	1.00 25.16	A
ATOM	787	CA	GLN	A	101	51.796	33.896	22.999	1.00 25.74	A
ATOM	788	CB	GLN			50.573	34.219	22.143	1.00 28.06	A
MOTA	789	CG	GLN			49.258	33.911	22.814	1.00 30.50 1.00 32.88	A A
ATOM	790	CD	GLN GLN			49.123 48.953	34.599 35.820	24.162 24.251	1.00 32.88	A
ATOM ATOM	791 792	OE1 NE2	GLN			49.202	33.813	25.221	1.00 33.04	A
ATOM	793	C			101	52.117	32.409	22.901	1.00 24.01	A
ATOM	794	Ô			101	52.280	31.881	21.807	1.00 24.25	A
MOTA	795	N			102	52.199	31.715	24.051	1.00 22.08	A
ATOM	796	CD	PRO	A	102	51.959	32.244	25.410	1.00 22.41	A
MOTA	797	CA	PRO	A	102	52.500	30.278	24.096	1.00 21.37	A
ATOM	798	CB			102	52.136	29.898	25.526	1.00 21.61	A
ATOM	799	CG	PRO		102	52.521	31.147	26.297	1.00 21.90 1.00 21.30	A A
ATOM	800	C			102	51.706	29.480	23.068	1.00 21.30	A
ATOM	801	O NT	PRO ASN		102 103	50.496 52.396	29.644 28.618	22.947 22.327	1.00 21.95	A
ATOM ATOM	802 803	N CA			103	51.749	27.802	21.305	1.00 17.69	A
ATOM	804	CB			103	52.040	28.379	19.913	1.00 17.99	A
ATOM	805	CG			103	50.899	28.162	18.929	1.00 18.28	A
ATOM	806	OD1			103	50.348	27.060	18.808	1.00 17.82	A
MOTA	807	ND2	ASN	A	103	50.549	29.223	18.204	1.00 17.71	A
ATOM	808	C			103	52.281	26.370	21.385	1.00 15.57	A
MOTA	809	0	ASN	A	103	53.000	26.012	22.310	1.00 14.67	A

ATOM	810	N	ILE A	104	51.918	25.565	20.397	1.00 15.80	A
ATOM	811	CA	ILE A		52.335	24.177	20.328	1.00 13.66	A
							20.888	1.00 15.40	A
ATOM	812	CB	ILE A		51.255	23.235			
MOTA	813	CG2	ILE A	104	51.589	21.792	20.539	1.00 13.82	A
ATOM	814	CG1	ILE A	104	51.132	23.421	22.400	1.00 17.40	A
MOTA	815	CD1	ILE A	104	50.129	22.494	23.047	1.00 18.65	A
ATOM	816	C	ILE A		52.588	23.775	18.896	1.00 14.36	A
MOTA	817	0		104	51.716	23.924	18.052	1.00 16.86	A
MOTA	818	N	LEU A	105	53.785	23.272	18.616	1.00 15.67	A
ATOM	819	CA	LEU A	105	54.090	22.822	17.272	1.00 15.52	A
ATOM	820	CB	LEU A	105	55.568	22.978	16.940	1.00 15.73	${f A}$
					56.058	24.391	16.649	1.00 20.75	A
MOTA	821	CG	LEU A						
ATOM	822	CD1	LEU A	1.05	57.400	24.298	15.919	1.00 20.19	A
ATOM	823	CD2	LEU A	105	55.030	25.141	15.791	1.00 21.31	A
MOTA	824	С	LEU A	105	53.709	21.362	17.202	1.00 15.97	A
ATOM	825	0	LEU A		53.968	20.589	18.133	1.00 14.11	${f A}$
							16.099	1.00 14.18	A
ATOM	826	N	ILE A		53.078	20.993			
ATOM	827	CA	ILE A	106	52.643	19.630	15.903	1.00 15.40	A
ATOM	828	CB	ILE A	106	51.122	19.576	15.636	1.00 15.11	A
ATOM	829	CG2	ILE A	106	50.661	18.135	15.592	1.00 12.46	A
					50.380	20.354	16.734	1.00 15.51	A
ATOM	830	CG1	ILE A						
ATOM	831	CD1	ILE A	106	48.862	20.413	16.565	1.00 12.83	A
ATOM	832	C	ILE A	106	53.381	19.011	14.725	1.00 16.48	A
ATOM	833	0	ILE A	106	53.484	19.607	13.651	1.00 17.37	${f A}$
ATOM	834	N	CYS A	107	53.900	17.811	14.944	1.00 17.86	A
					54.621	17.083	13.917	1.00 18.32	A
ATOM	835	CA		107					
ATOM	836	C	CYS A	107	53.886	15.776	13.663	1.00 18.29	A
ATOM	837	0	CYS A	107	53.846	14.909	14.533	1.00 18.13	A
ATOM	838	CB	CYS A	107	56.041	16.792	14.382	1.00 19.33	A
		SG		107	57.029	15.889	13.158	1.00 25.82	A
MOTA	839								
MOTA	840	N	LEU A	108	53.304	15.649	12.472	1.00 17.89	A
MOTA	841	CA	LEU A	108	52.556	14.456	12.088	1.00 18.82	A
MOTA	842	CB.	LEU A	108	51.330	14.850	11.252	1.00 20.17	A
ATOM	843	CG	LEU A	3.08	50.129	13.900	11.053	1.00 21.48	A
					49.623	14.049	9.624	1.00 20.62	A
MOTA	844	CD1							
ATOM	845	CD2	LEU A	108	50.493	12.458	11.316	1.00 18.40	A
MOTA	846	C	LEU A	108	53.445	13.538	11.252	1.00 19.49	A
ATOM	847	0	LEU A	108	53.841	13.892	10.144	1.00 20.39	\mathbf{A}
ATOM	848	N	VAL A	•	53.760	12.368	11.789	1.00 18.45	A
					54.586	11.398	11.087	1.00 19.04	A
ATOM	849	CA	VAL A						
ATOM	850	CB	VAL A	109	55.665	10.805	12.042	1.00 18.71	A
MOTA	851	CG1	VAL A	109	56.626	9.923	11.279	1.00 15.16	A
ATOM	852	CG2	VAL A	109	56.431	11.949	12.729	1.00 17.68	${f A}$
ATOM	853	C	VAL A	:	53.611	10.322	10.606	1.00 20.50	${f A}$
					53.115	9.516	11.393	1.00 21.55	A
ATOM	854	0	VAL A						
ATOM	855	N	ASP A	110	53.326	10.337	9.308	1.00 21.50	A
ATOM	856	CA	ASP A	110	52.376	9.407	8.700	1.00 21.95	A
ATOM	857	CB	ASP A	110	51.493	10.165	7.701	1.00 22.25	\mathbf{A}
ATOM	858	CG	ASP A	110	50.084	9.612	7.622	1.00 24.20	\mathbf{A}
					49.874	8.435	7.989	1.00 23.87	A
ATOM	859		ASP A						
MOTA	860	OD2	ASP A	110	49.182	10.356	7.182	1.00 25.94	A
MOTA	861	C	ASP A	110	53.059	8.240	7.985	1.00 21.53	A
MOTA	862	0	ASP A	110	54.273	8.254	7.782	1.00 18.80	A
ATOM	863	N	ASN A	111	52.254	7.245	7.603	1.00 23.78	A
		CA	ASN A		52.706	6.037	6.900	1.00 23.32	A
MOTA	864							1.00 24.67	
MOTA	865	CB	ASN A		53.046	6.360	5.437		A.
MOTA	866	CG	ASN A	111	53.181	5.102	4.575	1.00 31.76	A
ATOM	867	OD1	ASN A	111	52.291	4.240	4.567	1.00 31.05	${f A}$
MOTA	868	ND2			54.292	4.994	3.842	1.00 29.09	A
			ASN A		53.905	5.389	7.587	1.00 23.68	A
MOTA	869	C							
MOTA	870	0	ASN A		54.953	5.156	6.976	1.00 22.88	A
MOTA	871	N	ILE A	112	53.738	5.090	8.868	1.00 22.97	A
ATOM	872	CA	ILE A	112	54.797	4.473	9.646	1.00 20.73	A
ATOM	873	CB	ILE A		54.791	4.967	11.108	1.00 20.13	A
					55.979	4.363	11.864	1.00 15.53	A
ATOM	874	CG2							
MOTA	875	CG1			54.833	6.495	11.158	1.00 19.14	A
MOTA	876	CD1.	ILE A	112	54.671	7.058	12.575	1.00 20.42	A
ATOM	877	С	ILE A		54.658	2.960	9.699	1.00 22.54	A
ATOM	878	0	ILE A		53.605	2.436	10.054	1.00 22.65	A
								1.00 21.37	A
ATOM	879	N	PHE A		55.732	2.266	9.343		
MOTA	880	CA	PHE A		55.769	0.819	9.412	1.00 21.74	A
ATOM	881	CB	PHE A	113	54.742	0.167	8.483	1.00 21.64	A
ATOM	882	CG	PHE A		54.451	-1.252	8.850	1.00 21.22	A
			PHE A		53.528		9.856	1.00 20.25	A
MOTA	883	-DT	. EIID ∺	حه ملت بين			2.000		

ATOM	884	CD2	PHE	A	113	55.183	-2.296	8.285	1.00 20.76	A
MOTA	885	CE1	PHE	A	113	53.341	-2.848	10.302	1.00 19.85	A
ATOM	886	CE2			113	55.008	-3.607	8.721	1.00 20.75	A
ATOM	887	CZ			113	54.086	-3.887	9.735	1.00 21.24	A
ATOM	888	C			113	57.157 57.700	0.329 0.719	9.042 8.011	1.00 21.21 1.00 19.97	A A
ATOM ATOM	889 890	N			113 114	57.765	-0.509	9.893	1.00 19.97	A
ATOM	891	CD			114	59.118	-1.018	9.614	1.00 22.88	A
ATOM	892	CA			114	57.263	-1.040	11.170	1.00 23.38	A
ATOM	893	CB			114	58.340	-2.045	11.571	1.00 23.68	A
ATOM	894	CG	PRO	A	114	59.592	-1.435	10.984	1.00 23.26	A
ATOM	895	C	PRO	A	114	57.078	0.059	12.221	1.00 24.33	A
ATOM	896	0			114	57.571	1.174	12.054	1.00 24.35	A
ATOM	897	N			115	56.363	-0.247	13.319	1.00 24.59	A
ATOM	898	CD	PRO			55.579	-1.472	13.567	1.00 22.60	A
ATOM	899	CA	PRO			56.135 54.923	0.751 0.194	14.372 15.107	1.00 23.79 1.00 23.96	A A
ATOM ATOM	900 901	CB CG			115 115	55.129	-1.291	14.998	1.00 23.30	A
ATOM	902	C			115	57.337	0.996	15.289	1.00 24.97	A
ATOM	903	0			115	57.322	0.670	16.482	1.00 23.11	A
ATOM	904	N			116	58.380	1.573	14.705	1.00 24.77	A
ATOM	905	CA	VAL	A	116	59.607	1.902	15.423	1.00 24.05	A
ATOM	906	CB	VAL	A	116	60.733	0.881	15.135	1.00 26.45	A
ATOM	907	CG1	LAV	A	116	61.977	1.250	15.933	1.00 24.89	A
ATOM	908		VAL			60.267	-0.539	15.470	1.00 26.43	A
ATOM	909	C	VAL			60.043	3.254	14.875	1.00 24.47	A
MOTA	910	0	VAL			60.340	3.381	13.684	1.00 23.94	A
ATOM	911	N	VAL			60.088 60.472	4.269 5.577	15.728 15.239	1.00 22.43 1.00 22.18	A A
ATOM ATOM	912 913	CA CB	VAL VAL			59.247	6.277	14.565	1.00 22.18	A
ATOM	914		VAL			58.276	6.807	15.631	1.00 17.87	A
ATOM	915	CG2	VAL			59.710	7.387	13.653	1.00 19.98	A
ATOM	916	C	VAL			61.035	6.484	16.326	1.00 23.40	A
ATOM	917	0 /	VAL	A	117	60.743	6.323	17.512	1.00 22.77	A
MOTA	918	N	ASN	A	118	61.868	7.427	15.909	1.00 24.87	A
MOTA	919	CA	ASN	A	118	62.434	8.398	16.833	1.00 25.96	A
MOTA	920	CB	ASN			63.970	8.341	16.858	1.00 29.36	A
ATOM	921	CG	ASN			64.506	7.213	17.728	1.00 31.24	A
ATOM	922	OD1				63.885	6.833	18.722	1.00 34.20	A
ATOM	923	ND2	ASN ASN			65.679 61.989	6.694 9.746	17.374 16.312	1.00 34.04 1.00 24.87	A A
ATOM ATOM	924 925	С 0	ASN			62.298	10.112	15.177	1.00 24.07	A
ATOM	926	N	ILE			61.229	10.468	17.122	1.00 23.82	A
ATOM	927	CA	ILE			60.774	11.793	16.727	1.00 23.07	A
ATOM	928	CB	ILE	A	119	59.231	11.892	16.711	1.00 22.65	A
MOTA	929	CG2	ILE	A	119	58.797	13.197	16.051	1.00 18.01	A
MOTA	930	CG1	ILE			58.642	10.716	15.936	1.00 21.02	A
MOTA	931	CD1	ILE			57.135	10.714	15.921	1.00 21.88	A
ATOM	932	C			119	61.323	12.771	17.754	1.00 22.76	A
ATOM	933	0			119	61.013	12.680	18.940 17.303	1.00 22.92 1.00 23.11	A A
ATOM	934	N CA	THR		120	62.162 62.737	13.691 14.673	18.205	1.00 23.11	A
ATOM ATOM	935 936	CB			120	64.216	14.363	18.495	1.00 25.23	A
MOTA	937	OG1			120	64.921	14.199	17.258	1.00 26.55	A
ATOM	938	CG2			120	64.335	13.081	19.331	1.00 23.93	A
ATOM	939	C	THR	A	120	62.622	16.064	17.616	1.00 23.20	A
ATOM	940	0	THR	A	120	62.437	16.232	16.412	1.00 23.15	A
MOTA	941	N			121	62.725	17.069	18.470	1.00 22.54	A
MOTA	942	CA	_		121	62.619	18.432	17.998	1.00 21.37	A
MOTA	943	CB			121	61.563	19.196	18.791	1.00 19.43	A
MOTA	944	CG			121 121	60.173	18.679 19.179	18.616 17.703	1.00 18.76 1.00 19.96	A A
ATOM	945	CD2			121	59.191 58.002	18.454	17.703	1.00 18.06	A
ATOM ATOM	946 947	CE2 CE3			121	59.200	20.178	16.715	1.00 16.07	A
ATOM	947 948	CD1			121	59.567	17.694	19.330	1.00 18.18	A
ATOM	949	NE1	TRP		121	58.261	17.553	18.929	1.00 19.21	A
ATOM	950	CZ2	• • • • • • • • • • • • • • • • • • • •		121	56.827	18.694	17.210	1.00 16.20	A
ATOM	951	CZ3	TRP	A	121	58.036	20.419	16.000	1.00 16.43	A
ATOM	952	CH2	TRP		121	56.864	19.679	16.252	1.00 17.37	A
MOTA	953	C	TRP		121	63.927	19.178	18.097	1.00 22.88	A
ATOM	954	0	TRP		121	64.743	18.937	18.992	1.00 22.75	A
ATOM	955	N			122	64.109	20.100	17.164	1.00 23.24 1.00 22.66	A A
ATOM	956 957	CA			122 122	65.291 66.094	20.930 20.699	17.136 15.850	1.00 22.66	A A
MOTA	957	CB	חשת	ъ.	1. & &	00.054	20.033	T3.03U	<u></u>	A

ATOM	958	CG	LEU A	122	66.638	19.293	15.563	1.00 22.23	A
ATOM	959	CD1	LEU A	122	67.404	19.326	14.253	1.00 20.93	A
ATOM	960	CD2	LEU A	122	67.542	18.830	16.700	1.00 20.21	A
MOTA	961	C	LEU A	122	64.837	22.376	17.186	1.00 23.52	A
ATOM	962	0		122	63.830	22.752	16.572	1.00 21.74	A
ATOM	963	N	SER A		65.579	23.174	17.945	1.00 23.69	A
ATOM	964	CA	SER A		65.330	24.597	18.063	1.00 24.10	A
ATOM	965	CB	SER A		64.998	24.983	19.504	1.00 25.22	A
ATOM	966	OG G		123	64.735 66.664	26.373 25.200	19.591 17.650	1.00 25.55 1.00 24.79	A A
ATOM	967	C O	SER A		67.670	25.200	18.335	1.00 24.79	Ā
ATOM ATOM	968 969	N	ASN A		66.666	25.903	16.521	1.00 25.02	A
ATOM	970	CA		124	67.880	26.513	15.986	1.00 25.63	A
ATOM	971	CB	ASN A		68.351	27.676	16.868	1.00 24.46	A
ATOM	972	CG	ASN A		67.376	28.839	16.873	1.00 25.33	A
ATOM	973	OD1	ASN A	124	66.636	29.056	15.907	1.00 26.04	A
ATOM	974	ND2	ASN A	124	67.381	29.606	17.956	1.00 21.77	A
MOTA	975	C	ASN A	124	69.006	25.487	15.838	1.00 26.53	A
ATOM	976	0	ASN A		70.132	25.706	16.301	1.00 26.36	A
ATOM	977	N	GLY A		68.684	24.361	15.205	1.00 24.78	A
MOTA	978	CA	GLY A		69.669	23.326	14.964	1.00 26.09	A A
ATOM	979	C	GLY A		70.030 70.728	22.377 21.395	16.089 15.846	1.00 27.35 1.00 28.21	A A
ATOM	980	N O	GLY A HIS A	125	69.566	22.645	17.307	1.00 28.65	A
MOTA	981 982	CA		126	69.889	21.774	18.430	1.00 30.12	A
ATOM ATOM	983	CB	HIS A		70.816	22.507	19.408	1.00 32.68	A
ATOM	984	CG	HIS A		70.226	23.750	19.996	1.00 35.25	A
ATOM	985	CD2	HIS A		70.296	25.044	19.601	1.00 36.90	A
ATOM	986		HIS A		69.475	23.743	21.151	1.00 35.93	A
ATOM	987	CE1	HIS A	126	69.110	24.979	21.445	1.00 36.88	A
ATOM	988	NE2	HIS A	126	69.595	25.788	20.520	1.00 36.73	A
MOTA	989	C	HIS A	126	68.661	21.220	19.149	1.00 30.87	A
ATOM	990	0	HIS A		67.634	21.889	19.270	1.00 31.49	A
ATOM	991	N	SER A		68.789	19.990	19.635	1.00 30.93	A
ATOM	992	CA	SER A		67.697	19.286 17.889	20.302 20.714	1.00 33.08 1.00 33.91	A A
MOTA	993	CB	SER A		68.165 69.231	17.979	21.645	1.00 38.34	Ā
ATOM ATOM	994 995	OG C	SER A		67.050	19.971	21.501	1.00 32.98	A
ATOM	996	0	SER A		67.708	20.654	22.288	1.00 34.83	A
ATOM	997	N	VAL A		65.743	19.770	21.624	1.00 32.42	A
ATOM	998	CA	VAL A	128	64.960	20.325	22.716	1.00 31.29	A
MOTA	999	CB	VAL A	. 128	63.645	20.921	22.202	1.00 30.48	A
MOTA	1000	CG1			62.856	21.520	23.358	1.00 27.06	A
ATOM	1001	CG2			63.937	21.970	21.142	1.00 28.52	A
ATOM	1002	C	VAL A		64.645	19.183	23.669 23.237	1.00 32.28 1.00 32.80	A A
MOTA	1003	N	VAL A		64.275 64.786	18.093 19.437	24.965	1.00 32.80	A
MOTA MOTA	1004 1005	CA	THR A		64.546	18.411	25.981	1.00 33.70	A
ATOM	1005	CB	THR A		65.740	18.344	26.966	1.00 34.52	A
ATOM	1007	OG1			65.969	19.643	27.528	1.00 38.18	A
ATOM	1008	CG2	THR A		67.006	17.898	26.245	1.00 34.60	A
MOTA	1009	C	THR A	129	63.257	18.591	26.791	1.00 32.08	A
MOTA	1010	0	THR A	129	62.645	17.615	27.220	1.00 34.04	A
ATOM	1011	N	GLU A		62.843	19.835	26.993	1.00 28.85	A
MOTA	1012	CA	GLU A		61.639	20.119	27.762	1.00 26.09	A
ATOM	1013	CB	GLU A		61.926	21.236	28.770	1.00 28.58 1.00 32.87	A A
ATOM	1014	CG	GLU A		62.962 62.592	20.894 19.654	29.822 30.609	1.00 32.87	A
ATOM	1015 1016	CD OE1			61.392	19.475	30.907	1.00 37.85	A
ATOM ATOM	1017	OE2			63.501	18.865	30.941	1.00 36.29	A
ATOM	1018	C	GLU A		60.451	20.534	26.893	1.00 23.53	A
ATOM	1019	0	GLU A		60.629	21.166	25.859	1.00 19.76	A
ATOM	1020	N	GLY F	131	59.243	20.188	27.334	1.00 21.13	A
ATOM	1021	CA	GLY A	131	58.046	20.563	26.601	1.00 20.14	A
MOTA	1022	C	GLY A		57.693	19.684	25.421	1.00 20.64	A
MOTA	1023	0	GLY A		56.989	20.109	24.507	1.00 20.11	A
MOTA	1024	N	VAL A		58.164	18.447	25.444	1.00 18.28	A
ATOM	1025	CA	VAL A		57.899	17.527	24.355	1.00 20.08 1.00 20.35	A A
MOTA	1026	CB cca	VAL ? VAL ?		59.230 58.946	16.985 15.874	23.767 22.772	1.00 20.35	A
ATOM ATOM	1027 1028	CG1	_		60.006	18.114	23.093	1.00 20.17	Ā
ATOM	1026	CGZ	VAL I		57.027	16.340	24.786	1.00 20.06	A
ATOM	1020	0	VAL A		57.194	15.794	25.875	1.00 18.65	A
ATOM	1031	N	SER A	133	56.094	15.948	23.925	1.00 17.90	A

MOTA	1032	CA	SER A 133	55.238	14.802	24.215	1.00 18.16	A
MOTA	1033	CB	SER A 133	54.045	15.206	25.094	1.00 18.24	A
ATOM	1034	OG G	SER A 133	53.202 54.738	16.143 14.200	24.440 22.914	1.00 24.24 1.00 16.52	A A
ATOM ATOM	1035 1036	С О	SER A 133 SER A 133	54.876	14.794	21.843	1.00 16.18	A
ATOM	1037	N	GLU A 134	54.166	13.009	22.996	1.00 17.45	A
ATOM	1038	CA	GLU A 134	53.653	12.369	21.800	1.00 18.50	A
ATOM	1039	СВ	GLU A 134	54.797	11.661	21.050	1.00 22.31	A
ATOM	1040	CG	GLU A 134	55.475	10.513	21.801	1.00 24.62	A
ATOM	1041	CD	GLU A 134	56.610	9.859	20.992	1.00 28.65	A
MOTA	1042	OE1	GLU A 134	56.932	8.680	21.254	1.00 29.58	A
ATOM	1043	OE2	GLU A 134	57.188 52.523	10.521 11.389	20.099 22.087	1.00 27.96 1.00 18.44	A A
ATOM ATOM	1044 1045	C O	GLU A 134 GLU A 134	52.279	11.003	23.234	1.00 17.30	Ā
ATOM	1045	N	THR A 135	51.824	11.008	21.027	1.00 16.71	A
ATOM	1047	CA	THR A 135	50.733	10.059	21.119	1.00 15.49	A
MOTA	1048	CB	THR A 135	49.738	10.246	19.967	1.00 16.16	A
MOTA	1049	OG1	THR A 135	50.369	9.867	18.731	1.00 16.02	A
ATOM	1050	CG2	THR A 135	49.280	11.697	19.879	1.00 14.19	A
ATOM	1051	C	THR A 135	51.346	8.682	20.946	1.00 17.19 1.00 17.26	A A
MOTA	1052	O N	THR A 135	52.551 50.519	8.554 7.650	20.733 21.047	1.00 17.28	A
ATOM ATOM	1053 1054	N CA	SER A 136 SER A 136	51.001	6.297	20.818	1.00 15.92	A
ATOM	1055	CB	SER A 136	50.035	5.266	21.416	1.00 16.85	A
ATOM	1056	OG	SER A 136	49.756	5.532	22.781	1.00 18.22	A
ATOM	1057	C	SER A 136	50.967	6.187	19.294	1.00 15.84	A
MOTA	1058	0	SER A 136	50.715	7.169	18.596	1.00 17.25	A
MOTA	1059	N	PHE A 1.37	51.236	5.003	18.767	1.00 17.08	A
MOTA	1060	CA	PHE A 137	51.155	4.806	17.333 16.936	1.00 15.67 1.00 13.47	A A
ATOM	1061	CB CG	PHE A 137 PHE A 137	51.874 53.363	3.519 3.628	16.951	1.00 13.47	A
ATOM ATOM	1062 1063	CD1		54.037	4.255	15.907	1.00 15.82	A
ATOM	1064	CD2		54.100	3.112	18.010	1.00 15.21	A
ATOM	1065	CE1		55.427	4.367	15.918	1.00 15.72	A
ATOM	1066	CE2	PHE A 137	55.490	3.220	18.031	1.00 15.14	A
ATOM	1067	CZ	PHE A 137	56.152	3.848	16.983	1.00 14.35	A
ATOM	1068	C	PHE A 137	49.659	4.657	17.067	1.00 16.21 1.00 18.05	A A
ATOM	1069	0	PHE A 137	49.037 49.074	3.767 5.534	17.622 16.259	1.00 17.51	A
MOTA MOTA	1070 1071	N CA	LEU A 138 LEU A 138	47.648	5.433	15.953	1.00 19.20	A
ATOM	1071	CB	LEU A 138	47.017	6.822	15.800	1.00 20.80	A
ATOM	1073	CG	LEU A 138	46.809	7.688	17.044	1.00 23.47	A
ATOM	1074	CD1	LEU A 138	46.141	6.879	18.144	1.00 24.75	A
ATOM	1075	CD2		48.140	8.212	17.529	1.00 27.62	A
MOTA	1076	C	LEU A 138	47.490	4.637 4.862	14.658 13.698	1.00 18.41 1.00 16.16	A A
MOTA	1077	N O	LEU A 138 SER A 139	48.218 46.530	3.716	14.630	1.00 18.51	A
MOTA MOTA	1078 1079	CA	SER A 139	46.333	2.863	13.460	1.00 17.61	A
ATOM	1080	CB	SER A 139	45.481	1.656	13.836	1.00 18.17	A
MOTA	1081	OG	SER A 139	44.134	2.036	14.040	1.00 20.80	A
MOTA	1082	C	SER A 139	45.729	3.510	12.216	1.00 17.44	A
MOTA	1083	0	SER A 139	45.122	4.578	12.276	1.00 16.41	A
MOTA	1084	N	LYS A 140	45.908	2.822	11.088 9.778	1.00 18.56 1.00 18.37	A A
MOTA	1085	CA CB	LYS A 140 LYS A 140	45.402 46.543	3.237 3.751	8.895	1.00 21.60	A
MOTA MOTA	1086 1087	CG	LYS A 140	47.149	5.085	9.326	1.00 24.86	A
ATOM	1088	CD	LYS A 140	46.513	6.267	8.602	1.00 30.27	A
ATOM	1089	CE	LYS A 140	46.961	6.345	7.150	1.00 29.93	A
MOTA	1090	NZ	LYS A 140	48.440	6.349		1.00 30.14	A
ATOM	1091	C	LYS A 140	44.773	2.012	9.118	1.00 17.79	A
MOTA	1092	0	LYS A 140	45.106	0.878	9.458 8.160	1.00 17.76 1.00 18.54	A A
ATOM	1093	N	SER A 141 SER A 141	43.882 43.220	2.234 1.124	7.481	1.00 21.55	A
ATOM ATOM	1094 1095	CA CB	SER A 141	42.047		6.630	1.00 21.05	A
ATOM	1095		SER A 141	42.490		5.588	1.00 28.41	A
MOTA	1097	C	SER A 141	44.154		6.625	1.00 21.42	A
ATOM	1098	0	SER A 141	43.828		6.332	1.00 21.49	A
MOTA	1099	N	ASP A 142	45.311		6.226		A.
ATOM	1100	CA	ASP A 142	46.234		5.430 4.420		A A
MOTA	1101	CB	ASP A 142 ASP A 142	47.008 47.949				A
ATOM	1102 1103		ASP A 142 1 ASP A 142	47.949				A
ATOM ATOM	1103			48.799				A
ATOM	1105		ASP A 142	47.176			1.00 20.11	A
			,					

ATOM	1106	0	ASP A 142	48.127	-1.416	5.946	1.00 19.21	A
ATOM	1107	И	HIS A 143	46.885	-0.626	7.659	1.00 18.99	A
	1108	CA	HIS A 143	47.637	-1.295	8.706	1.00 17.27	A
ATOM				47.686	-2.792	8.409	1.00 16.45	A
ATOM	1109	CB		46.329	-3.396	8.190	1.00 18.33	A
ATOM	1110	CG	HIS A 143		-4.211	7.213	1.00 17.59	A
ATOM	1111	CD2	HIS A 143	45.860			1.00 17.33	A
MOTA	1112	ND1	HIS A 143	45.262	-3.151	9.032		A
ATOM	1113	CE1	HIS A 143	44.194	-3.786	8.580	1.00 19.46	
ATOM	1114	NE2	HIS A 143	44.529	-4.436	7.478	1.00 18.06	A
ATOM	1115	C	HIS A 143	49.019	-0.749	9.030	1.00 19.46	A
ATOM	1116	0	HIS A 143	49.812	-1.401	9.715	1.00 19.95	A
ATOM	1117	N	SER A 144	49.301	0.454	8.536	1.00 19.70	A
ATOM	1118	CA	SER A 144	50.542	1.141	8.852	1.00 20.18	A
ATOM	1119	CB	SER A 144	51.018	2.011	7.678	1.00 19.91	A
ATOM	1120	OG	SER A 144	50.099	3.044	7.364	1.00 23.64	A
ATOM	1121	C	SER A 144	50.109	2.018	10.034	1.00 19.40	A
ATOM	1122	0	SER A 144	48.970	1.906	10.499	1.00 19.70	A
	1123	N	PHE A 145	50.986	2.883	10.525	1.00 16.99	A
ATOM				50.614	3.728	11.649	1.00 16.06	A
ATOM	1124	CA			3.274	12.929	1.00 16.25	A
MOTA	1125	CB	PHE A 145	51.325			1.00 10.23	A
MOTA	1126	CG	PHE A 145	51.062	1.841	13.297		A
ATOM	1127	CD1		51.754	0.807	12.672	1.00 20.17	
ATOM	1128	CD2	PHE A 145	50.114	1.522	14.263	1.00 18.18	A
MOTA	1129	CEl	PHE A 145	51.505	-0.525	13.005	1.00 21.33	A
MOTA	1130	CE2	PHE A 145	49.856	0.193	14.606	1.00 19.50	A
MOTA	1131	CZ	PHE A 145	50.553	-0.831	13.975	1.00 20.23	A
MOTA	1132	C	PHE A 145	50.955	5.182	11.419	1.00 15.69	A
ATOM	1133	0	PHE A 145	51.548	5.538	10.404	1.00 16.69	A
ATOM	1134	N	PHE A 146	50.530	6.021	12.357	1.00 14.53	A
ATOM	1135	CA	PHE A 146	50.869	7.429	12.332	1.00 16.67	A
ATOM	1136	CB	PHE A 146	49.841	8.279	11.552	1.00 16.59	A
		CG	PHE A 146	48.535	8.528	12.259	1.00 15.25	A
ATOM	1137			48.370	9.644	13.071	1.00 15.42	A
MOTA	1138	CD1	_		7.708	12.019	1.00 16.06	A
ATOM	1139	CD2		47.433			1.00 17.50	A
MOTA	1140	CE1		47.123	9.952	13.629		A
ATOM	1141	CE2		46.180	8.003	12.571	1.00 16.80	
MOTA	1142	CZ	PHE A 146	46.023	9.126	13.375	1.00 17.47	A
MOTA	1143	С	PHE A 146	51.017	7.841	13.783	1.00 17.00	A
ATOM	1144	0	PHE A 146	50.345	7.308	14.661	1.00 19.50	A
ATOM	1145	N	LYS A 147	51.950	8.747	14.032	1.00 17.82	A
MOTA	1146	CA	LYS A 147	52.224	9.221	15.377	1.00 18.67	A
ATOM	1147	CB	LYS A 147	53.540	8.604	15.863	1.00 20.48	A
ATOM	1148	CG	LYS A 147	53.771	8.668	17.359	1.00 25.54	A
ATOM	1149	CD	LYS A 147	54.822	7.645	17.774	1.00 29.96	A
ATOM	1150	CE	LYS A 147	54.835	7.417	19.282	1.00 30.05	A
ATOM	1151	NZ	LYS A 147	55.740	6.291	19.643	1.00 33.05	A
ATOM	1152	C	LYS A 147	52.315	10.743	15.338	1.00 17.25	A
	1153	0	LYS A 147	52.716	11.320	14.329	1.00 19.15	A
ATOM			ILE A 148	51.932	11.391	16.428	1.00 15.47	A
ATOM	1154	N	ILE A 148	51.969	12.846	16.494	1.00 14.99	A
MOTA	1155	CA			13.424	16.642	1.00 15.37	A
ATOM	1156	CB	ILE A 148	50.529	14.932	16.740	1.00 14.06	A
MOTA	1157	CG2		50.566		15.426	1.00 16.41	A
MOTA	1158	CG:		49.689	13.025		1.00 18.41	A
MOTA	1159	CD:		48.223	13.325	15.550		
MOTA	1160	C	ILE A 148	52.829	13.271	17.682	1.00 17.07	A
MOTA	1161	O	ILE A 148	52.721	12.702	18.772	1.00 15.61	A
ATOM	1162	N	SER A 149	53.696	14.255	17.458	1.00 16.79	A
ATOM	1163	CA	SER A 149	54.570	14.757	18.514	1.00 17.66	A
ATOM	1164	CB	SER A 149	56.042	14.612	18.116	1.00 15.95	A
ATOM	1165	OG	SER A 149	56.900	14.956	19.190	1.00 17.31	A
MOTA	1166	C	SER A 149	54.239	16.225	18.763	1.00 18.34	A
ATOM	1167	0	SER A 149	53.854	16.949	17.842	1.00 18.33	A
ATOM	1168	N	TYR A 150	54.401	16.665	20.005	1.00 16.95	A
ATOM	1169	CA		54.085	18.040	20.362	1.00 17.59	A
		CB		52.893	18.057	21.310	1.00 17.57	A
MOTA	1170			51.679	17.314	20.797	1.00 18.52	A
ATOM	1171	CG			17.851	19.789	1.00 17.12	A
MOTA	1172			50.879		19.769	1.00 17.12	A
MOTA	1173	CE		49.733	17.182		1.00 18.32	A
MOTA	1174			51.313	16.078	21.345		
MOTA	1175			50.176	15.399	20.901		A
MOTA	1176	CZ	TYR A 150	49.391		19.900	1.00 17.92	A
MOTA	1177	OH	TYR A 150	48.275		19.457		A
MOTA	1178	C	TYR A 150	55.237	18.768		1.00 17.16	A
ATOM	1179	0	TYR A 150	55.953	18.207	21.847	1.00 19.65	A
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ATOM	1180	N	LEU	Z Z	151	55.409	20.029	20.649	1.00	17.01	A
ATOM	1181	CA	LEU			56.449	20.868	21.224	1.00	15.24	A
ATOM	1182	CB	LEU			57.540	21.182	20.197	1.00	16.33	A
ATOM	1183	CG	LEU			58.487	22.335	20.575	1.00	16.27	A
ATOM	1184	CD1	LEU			59.402	21.906	21.706	1.00	17.13	A
ATOM	1185	CD2	LEU			59.315	22.755	19.359	1.00	19.34	A
ATOM	1186	C	LEU			55.825	22.174	21.666	1.00	16.08	A
ATOM	1187	0	LEU			55.221	22.881	20.860	1.00	16.22	A
ATOM	1188	N	THR			55.952	22.497	22.945	1.00	16.84	A
ATOM	1189	CA	THR			55.428	23.765	23.424	1.00	18.70	A
ATOM	1190	CB	THR			55.283	23.799	24.946	1.00	20.14	A
ATOM	1191	OG1	THR			56.576	23.633	25.544	1.00	23.32	A
ATOM	1192	CG2	THR			54.355	22.694	25.419	1.00	18.36	A
ATOM	1193	C	THR			56.498	24.772	23.050	1.00	20.04	A
ATOM	1194	0	THR			57.689	24.448	23.034	1.00	20.72	A
ATOM	1195	N	LEU			56.085	25.986	22.735	1.00	20.63	A
ATOM	1196	CA			153	57.043	27.014	22.389	1.00	24.69	A
ATOM	1197	CB			153	57.579	26.794	20.960	1.00	24.19	A
ATOM	1198	CG			153	56.716	26.942	19.694	1.00	26.72	A
ATOM	1199	CD1			153	55.303	26.451	19.959	1.00	27.32	A
ATOM	1200	CD2			153	56.686	28.393	19.249	1.00	26.15	A
ATOM	1201	C			153	56.410	28.385	22.531	1.00	26.36	A
ATOM	1202	0			153	55.180	28.511	22.597	1.00	29.59	A
ATOM	1203	N			154	57.262	29.401	22.620	1.00	26.29	A
ATOM	1204	CA	LEU			56.830	30.787	22.729	1.00	26.89	A
MOTA	1205	CB	LEU			57.459	31.444	23.965		26.94	A
MOTA	1206	CG			154	56.966	32.833	24.407	1.00	28.58	A
ATOM	1207	CD1			154	55.507	32.755	24.864		24.43	A
MOTA	1208	CD2			154	57.845	33.342	25.549	1.00	27.14	A
MOTA	1209	C	LEU			57.337	31.458	21.456	1.00		A
ATOM	1210	o	LEU			58.538	31.689	21.304	1.00	30.73	A
ATOM	1211	N	PRO			56.428	31.773	20.518	1.00	30.57	A
ATOM	1212	CD	PRO			54.975	31.534	20.559	1.00	29.60	A
ATOM	1213	CA	PRO			56.806	32.412	19.254	1.00	31.63	A
ATOM	1214	CB	PRO			55.460	32.668	18.581	1.00	30.63	A
ATOM	1215	CG	PRO			54.612	31.552	19.087	1.00	28.73	A
ATOM	1216	C	PRO			57.639	33.688	19.370		33.58	A
ATOM	1217	0	PRO			57.322	34.593	20.136		33.98	A
ATOM	1218	N	SER			58.706	33.741	18.586	1.00	35.79	A
ATOM	1219	CA	SER			59.595	34.888	18.546	1.00	37.77	A
ATOM	1220	CB	SER			60.604	34.839	19.694	1.00		A
ATOM	1221	OG	SER			59.955	34.966	20.949	1.00		A
ATOM	1222	C	SER			60.332	34.841	17.222		38.83	A
ATOM	1223	0	SER			60.257	33.849	16.492	1.00		A
ATOM	1224	N	ALA			61.042	35.915	16.909		40.38	A
ATOM	1225	CA	ALA			61.796	35.972	15.670	1.00		A
ATOM	1226	СВ	ALA			61.822	37.401	15.148	1.00	40.36	A
ATOM	1227	C	ALA			63.214	35.466	15.918	1.00	39.65	A
MOTA	1228	0	ALA			64.058	35.504	15.021	1.00	39.72	A
ATOM	1229	N	GLU			63.463	34.984	17.135	1.00	39.12	A
MOTA	1230	CA	GLU	A	158	64.784	34.480	17.517	1.00	40.24	A
ATOM	1231	CB	GLU			65.082	34.808	18.988	1.00	44.21	A
ATOM	1232	CG	GLU	A	158	65.426	36.268	19.287	1.00	50.31	A
ATOM	1233	CD	GLU	A	158	64.204	37.174	19.356	1.00	55.36	A
ATOM	1234	OE1	GLU	A	158	64.353	38.351	19.765	1.00	55.75	A
ATOM	1235	OE2	GLU	A	158	63.095	36.712	19.002	1.00	58.12	A
ATOM	1236	С	GLU	A	158	65.005	32.979	17.303	1.00	38.02	A
ATOM	1237	0	GLU	A	158	66.130	32.493	17.419	1.00	36.30	A
ATOM	1238	N	GLU	A	159	63.950	32.234	17.002	1.00	35.79	A
MOTA	1239	CA	GLU	A	159	64.136	30.807	16.805	1.00	35.02	A
MOTA	1240	CB	GLU	A	159	63.949	30.066	18.135	1.00	36.97	A
ATOM	1241	CG	GLU	A	159	62.699	30.439	18.891	1.00	41.68	A
MOTA	1242	CD	GLU	A	159	62.717	29.933	20.323	1.00	44.82	A
MOTA	1243	OE1	GLU	A	159	62.819	28.705	20.527	1.00	46.62	A
MOTA	1244	OE2	GLU	A	159	62.631	30.767	21.248	1.00	47.25	A
MOTA	1245	C	GLU	A	159	63.277	30.162	15.735	1.00	32.21	A
ATOM	1246	0	GLU	A	159	62.147	30.574	15.473	1.00	32.05	A
MOTA	1247	N	SER	A	160	63.849	29.147	15.107	1.00	29.55	A
ATOM	1248	CA	SER	A	160	63.167	28.394	14.076	1.00	28.89	A
MOTA	1249	CB	SER	A	160	63.885	28.551	12.734	1.00	27.34	A
MOTA	1250	OG	SER			65.206	28.053	12.807		29.49	A
MOTA	1251	C	SER			63.241	26.957	14.565		27.42	A
ATOM	1252	0	SER			64.092	26.628	15.392		25.45	A
MOTA	1253	N	TYR	A	161	62.359	26.101	14.066	1.00	24.73	A

ATOM	1254	CA	TYR	A	161	62.359	24.725	14.517	1.00	24.26	A
MOTA	1255	CB	TYR			61.172	24.480	15.451		23.50	A
ATOM	1256	CG	TYR			60.935	25.593	16.434		24.01	A
ATOM	1257	CDI				60.255	26.748	16.052		26.02	A
ATOM	1258	CE1	TYR	A	161	60.009	27.774	16.959		27.93	A
MOTA	1259	CD2	TYR	A	161	61.374	25.491	17.753		24.78	A
ATOM	1260	CE2	TYR	A	161	61.136	26.514	18.674	1.00	25.93	A
ATOM	1261	CZ	TYR	A	161	60.450	27.650	18.270	1.00	27.56	A
MOTA	1262	OH	TYR	A	161	60.182	28.650	19.173	1.00	29.78	A
MOTA	1263	C	TYR	A	161	62.330	23.700	13.397	1.00	25.15	A
ATOM	1264	0	TYR	A	161	62.082	24.021	12.239	1.00	24.96	A
ATOM	1265	N	ASP	A	162	62.600	22.455	13.775	1.00	26.26	A
MOTA	1266	CA	ASP	A	162	62.598	21.331	12.858	1.00	26.94	A
ATOM	1267	CB	ASP		162	64.007	21.014	12.356	1.00	30.11	A
ATOM	1268	CG	ASP		162	64.548	22.067	11.434	1.00	32.85	A
MOTA	1269	OD1	ASP		162	64.075	22.138	10.277		33.31	A
ATOM	1270	OD2	ASP		162	65.443	22.819	11.874		33.08	A
ATOM	1271	C	ASP		162	62.122	20.117	13.613		25.87	A
ATOM	1272	0	ASP		162	62.449	19.947	14.789		24.38	A
ATOM	1273	N	CYS			61.352	19.277	12.935		23.95	A
ATOM	1274	CA	CYS		163	60.914	18.027	13.530		24.46	A
ATOM ATOM	1275 1276	С 0	CYS		163 163	61.916	17.043	12.938		22.46	A
ATOM	1277	CB	CYS		163	62.110 59.497	17.021 17.658	11.726 13.083		24.01 24.14	A
ATOM	1278	SG	CYS			58.931	16.101	13.836		30.35	A.
ATOM	1279	И	LYS			62.571	16.259	13.782		22.96	A A
ATOM	1280	CA	LYS			63.559	15.292	13.702		24.69	A
ATOM	1281	CB	LYS			64.867				27.54	A
ATOM	1282	CG	LYS			65.977	14.490	13.689		28.93	A
ATOM	1283	CD	LYS			67.179	14.643			32.03	A
ATOM	1284	CE	LYS			68.254	13.596	14.350		33.85	A
MOTA	1285	NZ	LYS			69.319	13.607			36.46	A
ATOM	1286	С	LYS	A		63.023	13.875	13.463		24.25	A
ATOM	1287	0	LYS	A	164	62.697	13.443	14.570	1.00	23.52	A
MOTA	1288	N	VAL	A	165	62.931	13.160	12.345	1.00	23.37	A
MOTA	1289	CA	VAL	A	165	62.415	11.797	12.344	1.00	24.06	A
MOTA	1290	CB	VAL	A	165	61.174	11.682	11.408	1.00	23.45	A
MOTA	1291	CG1	LAV	A	165	60.657	10.248	11.382	1.00	18.80	A
ATOM	1292	CG2	VAL	A	165	60.078	12.632	11.878	1.00	22.37	A
MOTA	1293	C	VAL	A		63.457	10.772	11.903	1.00	25.04	A
ATOM	1294	0	VAL			64.103	10.931	10.869		25.12	A
ATOM	1295	N	GLU			63.621	9.725	12.703		26.91	A
ATOM	1296	CA	GLU			64.556		12.383		28.84	A
MOTA	1297	CB	GLU			65.554		13.523	1.00		A
ATOM	1298	CG	GLU			66.382				36.90	A
ATOM	1299	CD OF1	GLU			67.247	9.356	15.147	1.00		A
ATOM ATOM	1300 1301	OE1 OE2	GLU			67.466 67.714	10.286	15.954	1.00	43.02	A.
ATOM	1302	C	GLU		•	63.739	8.206 7.369	15.301 12.183	1.00		A A
ATOM	1303	0	GLU			62.975	6.971	13.067	1.00		A
ATOM		N	HIS			63.910		11.029			A
ATOM	1305	CA	HIS			63.189	5.496	10.713	1.00		A
ATOM	1306	CB	HIS			61.838	5.833	10.084		30.90	A
ATOM	1307	CG	HIS			60.932	4.655	9.933		34.01	A
ATOM	1308	CD2	HIS	A	167	60.698	3.842	8.876	1.00		A
ATOM	1309	ND1	HIS	A	167	60.159	4.172	10.967	1.00	36.69	A
MOTA	1310	CE1	HIS	A	167	59.488	3.112	10.554	1.00	34.84	A
ATOM	1311	NE2	HIS	A	167	59.798	2.890	9.290	1.00	34.90	A
MOTA	1312	C	HIS	А	167	63.999	4.639	9.739	1.00	31.21	A
MOTA	1313	0	HIS	A	167	64.696	5.167	8.866	1.00	29.44	A
ATOM	1314	N	TRP	A	168	63.895	3.320	9.879	1.00	31.70	A
ATOM	1315	CA	TRP	A	168	64.625	2.402	9.006	1.00	31.76	A
MOTA	1316	CB	TRP			64.344	0.954	9.396	1.00		A
MOTA	1317	CG	TRP			64.735	0.650	10.797	1.00		A
ATOM	1318	CD2	TRP			64.115	-0.297	11.666	1.00		A
ATOM	1319		TRP			64.837	-0.288	12.878	1.00		A
ATOM	1320	CE3	TRP			63.017	-1.157	11.538	1.00		A
ATOM	1321	CD1	TRP			65.778	1.184	11.491	1.00		A
ATOM ATOM	1322	NE1	TRP			65.849	0.627	12.744	1.00		A.
ATOM ATOM	1323 1324	CZ2	TRP			64.498	-1.107	13.958	1.00		A.
ATOM	1324	CZ3 CH2	TRP		168	62.678 63.418	-1.970 -1.940	12.608 13.805	1.00 1.00		A. 20
ATOM	1326	CHZ	TRP			64.332	2.588	7.523	1.00		A A
ATOM	1327	0	TRP			65.190	2.314	6.682	1.00		A
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ATOM	1328	N	GLY	A	169	63	3.126	3	.049	7	.202	1.	00	34	.81	A
MOTA	1329	CA	GLY	A	169	62	2.760	3	.263	5	.810	1.	00	35	.23	A
ATOM	1330	C	GLY	A	169	63	3.267	4	.588	5	.266			37		A
ATOM	1331	0	GLY	A	169	62	2.907		.992		.162		00		. 65	A
MOTA	1332	N	LEU				1.100		.268		.049			39		A
ATOM	1333	CA	LEU				1.673		.555		.660		00		.10	A
ATOM	1334	CB	LEU				4.354		.626		.706				.47	A
MOTA	1335	CG	LEU				2.923		.143		.843		00		.66	A
MOTA	1336	CD1	LEU				2.790		.919		.142				.48	A
MOTA	1337	CD2	LEU				2.572		.017		.653		00		.65	A
ATOM	1338	C	LEU				5.183		.425		.556				.62	A
ATOM	1339	0	LEU				5.809		.762		.382		00		.45	A n
ATOM	1340	N	ASP		171		5.764		.066		.545		00		.98	A A
ATOM	1341	CA	ASP		171		8.211		.036		.350 .086		00		.99 .12	A A
ATOM	1342	CB	ASP		171 171		8.602 7.735		.466		.895				.30	A
ATOM	1343 1344	CG OD1	ASP ASP		171		6.520		.761		.936				.82	A
ATOM ATOM	1345	ODI ODI	ASP		171		8.271		.903		.917				.86	A
ATOM	1345	C C	ASP		171		8.836		.726		.554		00		.82	A
ATOM	1347	0	ASP		171		9.437		.093		.420		00		.88	A
ATOM	1348	N			172		8.673		.044		.585		00		.96	A
ATOM	1349	CA			172		9.192		.877		.659				.79	A
ATOM	1350	CB			172		9.986		.059		.084		00		.32	A
ATOM	1351	CG	LYS		172		1.074		.698		.075				.53	A
ATOM	1352	CD	LYS				1.799		.952		.571			57		A
ATOM	1353	CE	LYS		172		2.859		.621		.518				.22	A
ATOM	1354	NZ	LYS		172		3.912	10	.702	4	.038	1.	00	58	.32	A
ATOM	1355	C	LYS		172	6'	7.990	10	.419	7	.420	1.	00	46	.36	A
ATOM	1356	0	LYS	A	172	6	6.862	10	.381	6	.919	1.	00	44	.39	A
MOTA	1357	N	PRO	A	173	6	8.211	10	.920	8	.645	1.	00	44	.20	A
MOTA	1358	CD	PRO	A	173	6:	9.432	10	.866	9	.469	1.	00	44	.15	A
MOTA	1359	CA	PRO	A	173	6	7.089	11	.462	9	.410	1.	00	42	.74	A
ATOM	1360	CB	PRO	A	173	6	7.768	12	.050	10	.637	1.	00	42	.02	A
MOTA	1361	CG	PRO	A	173	6	8.887	11	.080		.872				.25	A
MOTA	1362	C	PRO	A	173		6.369		.517		.578				.09	A
ATOM	1363	0			173		7.002		.309		.877				.67	A
ATOM	1364	N			174		5.044		.502		.636				.80	A
MOTA	1365	CA			174		4.241		.457		.888				.58	A
ATOM	1366	СВ			174		2.894		.838		.522		00		.73	A
ATOM	1367	CG			174		2.202		.329		.251				.18	A 7
ATOM	1368	CD1	LEU		174		0.826		.691		.170				.20 .87	A A
MOTA	1369	CD2	LEU		174		2.093		.836		.785				.43	A
ATOM	1370	C			174 174		4.019 3.630		.514		.943				.68	A
ATOM ATOM	1371 1372	N O			175		4.284		.849		.255				.85	A
ATOM	1373	CA			175		4.098		.077		.012				.38	A
ATOM	1374	CB			175		5.400		.882		.074		00		.21	A
ATOM	1375	CG	LEU		175		6.425		7.502		.147		00		.82	A
ATOM	1376	CD1			175		5.838		7.768		.526		00		.32	A
ATOM	1377		LEU				6.819		.038		.008	1.	00	35	.37	A
MOTA	1378	C			175		3.020	17	7.898	8	.337	1.	.00	33	.09	A
ATOM	1379	0	LEU	A	175	6	3.080	18	3.137	7	.132	1.	.00	33	.84	A
ATOM	1380	N	LYS	A	176	6	2.023	18	3.312	9	.108	1.	.00	30	.14	A
ATOM	1381	CA	LYS	A	176	6	0.943	19	.119	8	.566	1.	.00	30	.03	A
MOTA	1382	CB	LYS	A	176	5	9.598	18	3.416	8	.772	1.	.00	30	.60	A
MOTA	1383	CG	LYS	A	176	5	8.463	19	0.049	8	.010	1.	.00	33	.60	A
MOTA	1384	CD	LYS	A	176	5	8.742	19	0.054	6	.508	1.	.00	37	.73	A
ATOM	1385	CE	LYS	A	176	5	8.869	17	7.642	5	.960				.37	A
MOTA	1386	NZ	LYS	A	176	5	9.075	17	7.629		.484				15	A
MOTA	1387	C	LYS	A	176	6	0.976		.457		.292				.62	A
ATOM	1388	0			176		0.764).524		.501				.68	A
ATOM	1389	N			. 177		1.238		L.520		.539				.72	A
ATOM	1390	CA			. 177		1.353		2.868		.088				.54	A
MOTA	1391	CB			. 177		2.284		3.691		1.195				.51	A
ATOM	1392	CG			177		2.485		5.097		3.663				.53	A
MOTA	1393				. 177		2.124		5.282		3.114				99	A
ATOM	1394				. 177		3.117		5.401		.849				.09	A 7
ATOM	1395				177		3.138		5.713		0.010				2.65	A A
ATOM	1396	NE2			177		2.542		7.271		3.971				2.04	A
MOTA	1397	C			177		0.059		3.654		3.304 3.549				7.66	A
MOTA	1398	O M	HIS		. 177 . 178		9.100		3.519 4.492		3.549).09	A
MOTA	1399 1400	N CA			178		8.926		5.350		0.340				3.43	A
ATOM ATOM	1400	CB			178		7.959		4.647		1.632				3.07	A
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ATOM	1402	CG	TRP	2\	178	56.681	25.422	11.851	1.00 25.25	A
ATOM	1403	CD2			178	56.476	26.518	12.761	1.00 21.68	A
ATOM	1404	CE2			178	55.138	26.942	12.611	1.00 20.86	A
	1405	CE3			178	57.292	27.178	13.688	1.00 20.72	A
ATOM					178	57.292	25.239	11.206	1.00 24.81	A
ATOM	1406	CD1				54.559	26.146	11.657	1.00 21.51	A
ATOM	1407	NE1			178			13.354	1.00 21.11	A
ATOM	1408	CZ2			178	54.598	27.999			
ATOM	1409	CZ3		A.	178	56.754	28.229	14.428	1.00 21.58	A
ATOM	1410	CH2			178	55.419	28.627	14.255	1.00 20.94	A.
MOTA	1411	C			178	59.425	26.628	11.348	1.00 36.30	A
MOTA	1412	0	TRP	A	178	60.314	26.591	12.195	1.00 36.91	A.
MOTA	1413	N	GLU	A	179	58.852	27.761	10.975	1.00 40.65	A
MOTA	1414	CA	GLU	A	179	59.240	29.029	11.587	1.00 45.62	A
MOTA	1415	CB	GLU	A	179	60.481	29.622	10.899	1.00 47.42	A
ATOM	1416	CG	GLU	A	179	60.323	29.868	9.404	1.00 52.77	A
ATOM	1417	CD	GLU	A	179	61.498	30.624	8.806	1.00 55.17	A
MOTA	1418	OE1	GLU	A	179	62.653	30.179	8.987	1.00 57.20	A
ATOM	1419	OE2	GLÜ	A	179	61.265	31.663	8.149	1.00 57.21	A
ATOM	1420	С	GLU	Α	179	58.074	30.001	11.489	1.00 46.47	A
ATOM	1421	0	GLU	A	179	57.322	29.983	10.513	1.00 45.49	${f A}$
ATOM	1422	N			180	57.898	30.855	12.509	1.00 47.97	A
ATOM	1423	CD			180	58.679	31.008	13.752	1.00 48.35	A
ATOM	1424	CA			180	56.789	31.810	12.460	1.00 49.45	A
		CB			180	56.763	32.372	13.880	1.00 49.39	A
ATOM	1425					58.214	32.358	14.266	1.00 48.65	A
ATOM	1426	CG	PRO				32.336	11.401	1.00 50.21	A
ATOM	1427	C	PRO			57.014	32.691		1.00 30.21	A
ATOM	1428	0	PRO			58.174		10.950		
MOTA	1429	OXT	PRO			56.030	33.578	11.043	1.00 50.90	A
MOTA	1430	CB	SER		3	67.953	-2.426	7.203	1.00 59.72	В
ATOM	1431	OG	SER		3	68.517	-3.384	6.321	1.00 60.71	В
MOTA	1432	C	SER	В	3	68.164	-3.822	9.277	1.00 57.49	В
MOTA	1433	0	SER	В	3	68.117	-4.879	8.642	1.00 57.32	B -
ATOM	1434	N	SER	В	3	70.072	-2.418	8.486	1.00 59.35	В
MOTA	1435	CA	SER	В	3	68.586	-2.517	8.597	1.00 58.84	В
MOTA	1436	N	PRO	В	4	67.855	-3.763	10.585	1.00 55.71	В
ATOM	1437	CD	PRO	В	4	67.914	-2.580	11.463	1.00 54.97	В
MOTA	1438	CA	PRO	В	4	67.438	-4.952	11.338	1.00 53.72	В
ATOM	1439	СВ	PRO	В	4	67.457	-4.467	12.787	1.00 54.71	В
MOTA	1440	CG	PRO	В	4	67.095	-3.021	12.660	1.00 54.93	В
ATOM	1441	С	PRO	В	4	66.069	-5.487	10.918	1.00 51.05	В
ATOM	1442	0	PRO		4	65.240	-4.753	10.379	1.00 50.96	В
ATOM	1443	N	GLU		5	65.843	-6.773	11.165	1.00 47.90	В
ATOM	1444	CA	GLU			64.581		10.810	1.00 45.24	В
ATOM	1445	CB	GLU			64.811		10.489	1.00 48.23	В
		CG	GLU			65.603	-9.656	11.545	1.00 54.54	В
ATOM	1446		GLU			65.896		11.140	1.00 57.83	В
ATOM	1447	CD					-11.317	10.024	1.00 59.67	В
ATOM	1448	OE1	GLU							В
ATOM	1449	OE2	GLU				-12.020	11.941	1.00 59.33	
ATOM	1450	C	GLU			63.548		11.920	1.00 40.85	В
ATOM	1451	0	GLU			63.876		13.105	1.00 40.81	В
ATOM	1452	N	ASP	В	6	62.294		11.532	1.00 36.03	B -
MOTA	1453	CA	ASP	B	6	61.223	-6.936	12.508	1.00 32.11	B
MOTA	1454	CB	ASP	В	6	60.833	-5.460	12.616	1.00 29.96	В
ATOM	1455	CG	ASP	В	6	59.933	-5.171	13.798	1.00 27.91	B
ATOM	1456	OD1	ASP	В	6	59.280	-4.110	13.785	1.00 29.62	В
ATOM	1457	OD2	ASP	В	6	59.884	-5.982	14.745	1.00 29.86	В
MOTA	1458	C	ASP	В	6	60.014	-7.766	12.077	1.00 29.68	В
MOTA	1459	0	ASP	В	6	59.676	-7.802	10.899	1.00 29.14	В
ATOM	1460	N	PHE	В	7	59.380	-8.438	13.032	1.00 27.77	В
ATOM	1461	CA	PHE			58.193	-9.249	12.765	1.00 28.11	В
ATOM	1462	CB	PHE			58,453		13.161	1.00 29.55	В
ATOM	1463	CG	PHE				-11.385	12.282	1.00 31.06	В
ATOM	1464	CD1					-11.766	10.989	1.00 29.85	В
							-11.603	12.730	1.00 32.21	В
MOTA	1465	CD2				60.761		10.145	1.00 32.21	В
ATOM	1466		PHE					11.897	1.00 33.73	B
ATOM	1467	CE2				61.719			1.00 34.27	B
ATOM	1468	CZ	PHE			61.373		10.599		В
ATOM	1469	C	PHE			57.032		13.562	1.00 26.58	
ATOM	1470	0	PHE			57.046		14.794	1.00 25.72	В
MOTA	1471	N	VAL			56.023		12.849	1.00 25.17	В
ATOM	1472	CA	VAL			54.891		13.493	1.00 23.46	В
MOTA	1473	CB	VAL			54.670		12.871	1.00 21.55	В
MOTA	1474	CG1	. VAL	E	8	53.573		13.612	1.00 21.83	В
MOTA	1475	CG2	VAL	E	8	55.975	-5.342	12.895	1.00 21.30	В

VAL B 53.556 -8.255 13.467 1.00 24.08 MOTA 1476 C 8 \mathbf{B} В MOTA 1477 0 VAL B 53.204 -8.912 12.491 1.00 23.46 1478 \mathbf{N} TYR B 52.804 -8.127 14.554 1.00 23.26 В MOTA TYR B В ATOM 1479 CA 51.493 -8.74714.619 1.00 23.18 ATOM 1480 CB TYR B 51.510 -9.978 15.520 1.00 23.12 B TYR B В ATOM 1481 CG 50.231 -10.786 15.465 1.00 24.54 14.722 CD1 TYR B 50.158 -11.962 1.00 26.50 В ATOM 1482 CE1 TYR B 14.716 \mathbb{B} ATOM 1483 49.000 -12.743 1.00 25.08 ATOM 1484 CD2 TYR B 49.108 -10.399 16.190 1.00 22.88 \mathbf{B} TYR B B CE2 47.948 -11.165 16.188 1.00 23.91 ATOM 1485 TYR B 47.902 -12.342 \mathbb{B} 1486 CZ9 15.455 1.00 24.87 ATOM 9 46.780 -13.140 1.00 25.45 B ATOM 1487 OH TYR B 15.501 В ATOM 1488 C TYR B 9 50.509 -7.72315.163 1.00 21.33 1.00 22.92 В 1489 TYR B 9 50.798 -7.028 16.133 ATOM 0 14.521 1.00 19.98 \mathbf{B} MOTA 1490 GLN B 10 49.353 -7.622 N CA GLN B 48.326 -6.687 14.952 1.00 19.52 В ATOM 1491 10 В **ATOM** 1492 CB GLN B 10 48.171 -5.523 13.962 1.00 19.13 В 13.509 ATOM 1493 CG GLN B 10 49.433 -4.8101.00 19.33 1.00 17.96 В -3.708 12.499 MOTA 1494 CD GLN B 10 49.117 \mathbf{B} ATOM 1495 OE1 GLN B 10 48.336 -2.802 12.783 1.00 18.49 1.00 19.41 В GLN B -3.790 \cdot 11.316 MOTA 1496 NE2 10 49.715 В C -7.37515.029 1.00 19.74 1497 GLN B 10 46.967 ATOM 1498 GLN B 10 46.626 -8.227 14.192 1.00 18.98 В MOTA 0 1.00 19.06 B PHE B -6.996 16.040 MOTA 1499 \mathbf{N} 11 46.195 PHE B 44.842 -7.48716.182 1.00 16.54 В MOTA 1500 CA 1.1 1501 PHE B 1.00 17.48 В CB 11 44.668 -8.45417.336 MOTA B MOTA 1502 CG PHE B 11 43.237 -8.847 17.544 1.00 16.17 1.00 17.49 -9.604 16.582 В CD1 PHE B 11 42.570 ATOM 1503 B 18.656 CD2 PHE B 11 42.536 -8.406 1.00 14.41 ATOM 1504 CE1 PHE B 41.219 -9.913 16.725 1.00 18.03 \mathbf{B} MOTA 1505 11 В 18.814 1.00 16.34 ATOM 1506 CE2 PHE B 11 41.191 -8.708 В PHE B 40.528 -9.463 17.845 1.00 17.60 1507 CZ11 MOTA -6.271 \mathbf{B} C PHE B 43.984 16.450 1.00 18.14 MOTA 1508 11 В 1509 PHE B 11 44.241 -5.506 17.386 1.00 15.63 MOTA 0 В 1.00 17.33 LYS B 42.961 -6.094 15.625 MOTA 1510 N12 В LYS B -4.958 15.770 1.00 17.63 1511 12 42.082 ATOM CA В LYS B -4.06714.536 1.00 18.71 ATOM 1512 CB 12 42.188 \mathbb{B} 43.599 14.192 1.00 15.90 ATOM 1513 CG LYS B 12 -3.642 В 12.871 1.00 17.33 LYS B 12 43.602 -2.909MOTA 1514 CD 12.570 1.00 18.72 В LYS B 12 44.946 -2.297ATOM 1515 CE 1.00 20.93 В NZLYS B 12 44.838 -1.45011.340 MOTA 1516 \mathbf{B} -5.387 15.968 1.00 18.92 C LYS B 12 40.632 ATOM 1517 LYS B В 12 40.041 -6.050 15.109 1.00 17.25 1518 0 MOTA \mathbf{B} GLY B 40.076 -5.002 17.114 1.00 17.59 1519 N ATOM \mathbf{B} MOTA 1520 CA GLY B 13 38.701 -5.322 17.430 1.00 19.88 1.00 20.12 \mathbf{B} GLY B 37.874 MOTA 1521 C 13 -4.11317.064 В 37.515 -3.309 17.923 1.00 21.08 1522 0 GLY B 13 ATOM В ATOM 1523 NMET B 14 37.561 -4.00015.779 1.00 20.42 1.00 22.96 \mathbf{B} 14 36.817 -2.866 15.262 1524 CA MET B ATOM 13.866 1.00 23.02 В MET B 37.334 -2.554 ATOM 1525 CB 14 1.00 23.58 1526 MET B 14 38.846 -2.485 13.820 В ATOM CG 12.191 1.00 26.23 В 1527 MET B 39.449 -2.095 MOTA SD 14 12.182 В 1528 MET B 39.260 -0.318 1.00 25.78 ATOM CE14 35.295 -2.997 15.242 1.00 23.12 В MOTA 1529 C MET B 14 15.081 \mathbf{B} ATOM 1530 0 MET B 14 34.751 -4.0891.00 24.36 В 34.628 15.427 1531 N CYS B 15 -1.860 1.00 24.04 ATOM 1.00 24.91 В 33.173 -1.76815.433 ATOM 1532 ÇA CYS B 15 \mathbf{B} C 15 32.808 -0.58714.547 1.00 25.49 ATOM 1533 CYS B В 33.369 0.504 14.700 1.00 23.97 ATOM 1534 0 CYS B 15 1.00 26.02 32.630 -1.48916.847 В 1535 CYS B 15 MOTA CB 1536 32.691 -2.831 18.084 1.00 33.69 \mathbf{B} ATOM SG CYS B 15 31.871 -0.805 13.630 1.00 25.87 \mathbf{B} ATOM 1537 NTYR B 16 В 31.413 0.244 12.724 1.00 25.59 MOTA 1538 CA TYR B 16 31.539 -0.223 11.274 В 1539 TYR B 1.00 24.73 ATOM CB 16 32.958 \mathbf{B} ATOM 1540 TYR B -0.575 10.879 1.00 26.05 CG 16 \mathbf{B} 33.523 11.239 CD1 TYR B -1.7951.00 22.96 ATOM 1541 16 В 34.843 -2.102 10.904 1.00 25.81 ATOM 1542 CE1 TYR B 16 В ATOM CD2 TYR B 33.748 0.334 10.171 1.00 25.30 1543 16 B TYR B 35.066 0.041 9.835 1.00 25.12 ATOM 1544 CE2 16 В 10.202 ATOM 1545 TYR B 16 35.607 -1.1761.00 26.66 CZ \mathbf{B} 36.908 -1.4639.868 1.00 29.22 ATOM 1546 OH TYR B 16 \mathbf{B} ATOM 1547 C TYR B 16 29.960 0.575 13.045 1.00 26.48 В 29.113 -0.315 13.091 ATOM 1548 0 TYR B 16 1.00 26.41 В 29.684 1.859 13.266 ATOM 1549 N PHE B 17 1.00 27.76

ATOM	1550	CA	PHE	В	17	28.346	2.338	13.613	1.00 29.09	В
ATOM	1551	CB	PHE	B	17	28.382	3.047	14.967	1.00 28.08	В
ATOM	1552	CG	PHE	В	17	28.885	2.194	16.091	1.00 28.21	В
ATOM	1553	CD1	PHE		17	28.056	1.253	16.693	1.00 27.20	В
ATOM	1554		PHE		17	30.188	2.340	16.558	1.00 26.60	В
								17.752	1.00 28.13	В
MOTA	1555	CEI	PHE		17	28.519	0.470			
MOTA	1556	CE2	PHE		17	30.662	1.565	17.610	1.00 25.62	В
MOTA	1557	CZ	PHE	В	17	29.828	0.629	18.210	1.00 26.17	В
MOTA	1558	Ĉ	PHE	В	17	27.772	3.318	12.592	1.00 30.71	В
ATOM	1559	0	PHE	В	17	28.452	4.239	12.155	1.00 31.05	В
ATOM	1560	N	THR		18	26.506	3.125	12.237	1.00 33.51	В
ATOM	1561	CA	THR		18	25.831	4.005	11.291	1.00 36.95	В
						25.797	3.395	9.875	1.00 37.23	В
ATOM	1562	CB	THR		18					
ATOM	1563	OG1	THR		18	27.133	3.105	9.447	1.00 40.77	B
ATOM	1564	CG2	THR	В	18	25.171	4.369	8.891	1.00 38.43	В
ATOM	1565	C	THR	В	18	24.398	4.273	11.753	1.00 38.56	В
ATOM	1566	0	THR	В	18	23.671	3.351	12.131	1.00 38.36	B
ATOM	1567	N	ASN	В	19	24.007	5.544	11.726	1.00 39.80	В
ATOM	1568	CA	ASN		19	22.668	5.961	12.132	1.00 41.35	В
ATOM	1569	CB	ASN		19	21.638	5.465	11.110	1.00 41.21	В
							6.190	11.223	1.00 42.85	В
MOTA	1570	CG	ASN		19	20.311				
ATOM	1571	OD1	ASN		19	20.271	7.378	11.548	1.00 42.24	B
MOTA	1572	ND2	ASN	В	19	19.219	5.485	10.937	1.00 42.57	В
ATOM	1573	C	ASN	В	19	22.352	5.416	13.521	1.00 42.37	В
ATOM	1574	0	ASN	В	19	21.540	4.503	13.673	1.00 43.36	В
ATOM	1575	N	GLY		20	22.997	5.989	14.533	1.00 42.56	В
ATOM	1576	CA	GLY		20	22.790	5.535	15.894	1.00 43.89	В
		C	GLY		20	23.293	4.110	16.031	1.00 45.10	В
ATOM	1577							15.646	1.00 44.28	В
ATOM	1578	0	GLY		20	24.421	3.807			
MOTA	1579	N	THR	В	21	22.458	3.232	16.575	1.00 46.37	B
MOTA	1580	CA	THR	В	21	22.824	1.832	16.738	1.00 47.42	B
ATOM	1581	CB	THR	В	21	22.667	1.373	18.199	1.00 48.57	В
ATOM	1582	OG1	THR	В	21	21.438	1.885	18.731	1.00 49.14	В
ATOM	1583	CG2	THR		21	23.843	1.856	19.043	1.00 47.59	В
		C	THR		21	21.958	0.947	15.846	1.00 48.74	В
ATOM	1584						-0.276	16.016	1.00 48.04	В
ATOM	1585	0	THR		21	21.925				
MOTA	1586	N	GLU		22	21.253	1.570	14.902	1.00 48.57	В
ATOM	1587	CA	GLU	В	22	20.405	0.822	13.979	1.00 48.90	В
MOTA	1588	CB	GLU	В	22	19.741	1.745	12.957	1.00 52.60	В
ATOM	1589	CG	GLU	В	22	18.669	2.667	13.493	1.00 58.06	В
ATOM	1590	CD	GLU	В	22	17.862	3.297	12.368	1.00 62.27	В
ATOM	1591	OE1	GLU		22	17.027	4.185	12.648	1.00 63.99	В
					22	18.065	2.894	11.199	1.00 64.70	В
ATOM	1592	OE2	GLU						1.00 46.38	B
ATOM	1593	C	GLU		22	21.285	-0.156	13.229		
ATOM	1594	0	GLU	В	22	21.029	-1.356	13.209	1.00 45.52	B
ATOM	1595	N	ARG	В	23	22.324	0.379	12.601	1.00 45.42	В
ATOM	1596	CA	ARG	В	23	23.260	-0.438	11.844	1.00 44.59	В
ATOM	1597	CB	ARG	В	23	23.423	0.127	10.422	1.00 45.69	В
ATOM	1598	CG	ARG		23	22.169	-0.062	9.554	1.00 49.95	В
			ARG		23	22.406	0.237	8.074	1.00 53.34	В
ATOM	1599	CD						7.708	1.00 55.57	B
ATOM	1600	NE	ARG		23	22.153	1.632			
ATOM	1601	CZ	ARG		23	20.949	2.200	7.700	1.00 57.20	В
MOTA	1602	NH1	ARG	В	23	19.878	1.495	8.042	1.00 58.09	B
ATOM	1603	NH2	ARG	В	23	20.813	3.471	7.340	1.00 56.82	В
ATOM	1604	C	ARG	В	23	24.606	-0.534	12.567	1.00 40.56	В
ATOM	1605	0	ARG	В	23	25.306	0.459	12.748	1.00 41.15	В
ATOM	1606	N	VAL		24	24.944	-1.743	12.995	1.00 38.17	В
ATOM		CA	VAL		24	26.191	-1.996	13.708	1.00 34.88	В
	1607					25.931	-2.314	15.200	1.00 34.41	В
ATOM	1608	CB	VAL		24					В
MOTA	1609	CG1			24	27.251	-2.526	15.918	1.00 35.28	
ATOM	1610	CG2	VAL	В	24	25.146	-1.190	15.852	1.00 34.70	В
ATOM	1611	C	VAL	В	24	26.909	-3.194	13.100	1.00 32.34	В
ATOM	1612	0	VAL	В	24	26.287	-4.214	12.812	1.00 33.23	В
ATOM	1613	N	ARG		25	28.217	-3.076	12.898	1.00 30.18	В
ATOM	1614	CA	ARG		25	28.970	-4.194	12.354	1.00 26.97	В
						29.225	-4.022	10.852	1.00 27.67	B
ATOM	1615	CB	ARG		25					В
MOTA	1616	CG	ARG		25	29.400	-5.362	10.170	1.00 29.58	
ATOM	1617	CD	ARG	B	25	30.406	-5.363	9.052	1.00 31.26	В
ATOM	1618	NE	ARG	В	25	30.058	-4.454	7.974	1.00 33.12	В
ATOM	1619	ÇZ	ARG	В	25	30.415	-4.631	6.705	1.00 32.27	В
ATOM	1620	NH1			25	31.124	-5.695	6.346	1.00 31.13	В
ATOM	1621	NH2			25	30.087	-3.726	5.799	1.00 30.62	В
					25 25	30.305	-4.402	13.065	1.00 24.10	В
ATOM	1622	C	ARG			31.095		13.225	1.00 24.16	В
ATOM	1623	0	ARG	, R	25	21.032	-3.477	13.443	1.00 22.30	

ATOM	1624	N	LEU	В	26	30.551	-5.630	13.495	1.00 22.65	В
ATOM	1625	CA	LEU	В	26	31.801	-5.942	14.163	1.00 22.38	В
MOTA	1626	CB	LEU	В	26	31.558	-6.888	15.345	1.00 20.25	В
MOTA	1627	CG		В	26	32.795	-7.389	16.100	1.00 19.86	В
ATOM	1628	CD1	LEU		26	32.452	-7.613	17.568	1.00 22.49	B
ATOM ATOM	1629 1630	CD2 C	LEU		26 26	33.304 32.726	-8.665 -6.591	15.464 13.150	1.00 18.43 1.00 21.50	B B
ATOM	1631	0		В	26	32.720	-7.402	12.342	1.00 22.83	В
ATOM	1632	N	VAL		27	33.998	-6.208	13.177	1.00 21.29	В
ATOM	1633	CA	VAL		27	34.984	-6.780	12.270	1.00 20.66	В
MOTA	1634	CB	VAL	В	27	35.178	-5.911	11.004	1.00 20.59	В
MOTA	1635	CG1	VAL	В	27	36.169	-6.576	10.069	1.00 19.45	В
MOTA	1636	CG2	VAL		27	33.849	-5.696	10.297	1.00 22.37	В
ATOM	1637	C	VAL		27	36.330	-6.885	12.988	1.00 22.39	В
ATOM	1638	0	VAL		27	37.046	-5.889	13.135	1.00 22.63	В
ATOM ATOM	1639 1640	N CA	SER SER		28 28	36.673 37.947	-8.083 -8.259	13.450 14.130	1.00 21.32 1.00 21.51	B B
ATOM	1641	CB	SER		28	37.831	-9.284	15.275	1.00 19.72	В
ATOM	1642	OG	SER		28	37.542	-10.581	14.819	1.00 24.33	В
ATOM	1643	C	SER		28	38.954	-8.693	13.074	1.00 21.25	В
ATOM	1644	0	SER	В	28	38.661	-9.537	12.229	1.00 19.44	В
ATOM	1645	N	ARG	В	29	40.137	-8.089	13.106	1.00 20.61	В
ATOM	1646	CA	ARG	В	29	41.158	-8.402	12.115	1.00 19.66	В
ATOM	1647	CB	ARG		29	41.418	-7.169	11.230	1.00 19.91	В
ATOM	1648	CG	ARG		29	40.178	-6.407	10.754	1.00 16.79	В
ATOM	1649	CD	ARG		29 29	40.608	-5.121 -4.318	10.031 9.553	1.00 18.10 1.00 19.38	B B
ATOM ATOM	1650 1651	NE CZ	ARG ARG		29	38.738	-4.510	9.553 8.497	1.00 20.62	В
MOTA	1652	NH1	ARG		29	38.983	-5.714	7.789	1.00 19.50	В
ATOM	1653	NH2	ARG		29	37.736	-3.822	8.149	1.00 21.90	В
ATOM	1654	C	ARG	В	29	42.482	-8.833	12.738	1.00 18.57	В
ATOM	1655	0	ARG	В	29	43.024	-8.121	13.584	1.00 19.40	В
ATOM	1656	N	SER		30	42.991	-9.995	12.326	1.00 18.99	В
ATOM	1657	CA	SER		30	44.284	-10.501	12.797	1.00 21.66	В
ATOM	1658	CB	SER		30	44.241	-12.015 -12.352	13.023 14.106	1.00 22.77 1.00 26.81	B B
ATOM ATOM	1659 1660	OG C	SER SER		30 30	45.265		11.673	1.00 23.37	В
ATOM	1661	0	SER		30	45.055		10.522	1.00 21.31	В
ATOM	1662	N	ILE		31	46.338	-9.450	12.009	1.00 24.76	В
ATOM	1663	CA	ILE	В	31	47.298	-8.998	10.999	1.00 24.33	В
ATOM	1664	CB	ILE	В	31	47.341	-7.440	10.958	1.00 25.20	В
ATOM	1665	CG2	ILE		31	47.982		9.672	1.00 23.24	В
MOTA	1666		ILE		31	45.934	-6.857	11.106	1.00 26.96	В
ATOM	1667	CD1			31	45.032 48.741	-7.136 -9.460	9.947 11.187	1.00 31.25 1.00 23.98	B B
ATOM ATOM	1668 1669	С О	ILE		31 31	49.298	-9.318	12.272	1.00 23.38	В
ATOM	1670	И	TYR		32	49.345	-9.993	10.123	1.00 25.50	B
ATOM	1671	CA	TYR		32		-10.405	10.162	1.00 26.21	В
ATOM	1672	CB	TYR		32	50.965	-11.764	9.492	1.00 28.46	В
ATOM	1673	CG	TYR	В	32	52.406	-12.224	9.544	1.00 31.10	В
MOTA	1674	CD1	TYR		32			10.765	1.00 32.47	В
ATOM	1675		TYR		32		-12.780	10.827	1.00 34.69	В
ATOM	1676	CD2	TYR		32		-12.424	8.375 8.422	1.00 33.60 1.00 34.50	B B
ATOM ATOM	1677 1678	CE2	TYR TYR		32 32		-12.795 -12.965	9.654	1.00 35.65	В
ATOM	1679	OH	TYR		32	56.438	-13.281	9.717	1.00 37.73	В
ATOM	1680	C	TYR		32	51.478	-9.307	9.384	1.00 25.67	В
ATOM	1681	Ō	TYR		32	51.273	-9.140	8.174	1.00 24.75	В
MOTA	1682	N	ASN	В	33	52.319	-8.559	10.094	1.00 25.63	В
MOTA	1683	CA	ASN	B	3 3	53.036	-7.416	9.526	1.00 24.95	В
ATOM	1684	CB	ASN		33	53.955	-7.848	8.379	1.00 23.75	В
ATOM	1685	CG	ASN		33	55.171	-8.615	8.878	1.00 24.11 1.00 25.42	B B
MOTA	1686	OD1			33 33	55.803 55.506	-8.223 -9.708	9.861 8.204	1.00 25.42 1.00 25.18	В
ATOM ATOM	1687 1688	ND2 C	ASN		33	51.990	-6.392	9.070	1.00 25.11	B
ATOM	1689	0	ASN		33	51.491	-5.618	9.893	1.00 26.06	В
ATOM	1690	√N	ARG		34	51.652	-6.375	7.786	1.00 25.75	В
MOTA	1691	CA	ARG		34	50.631	-5.449	7.296	1.00 27.64	В
MOTA	1692	CB	ARG		34	51.244	-4.362	6.408	1.00 27.74	В
ATOM	1693	CG	ARG		34	51.972	-3.257	7.158	1.00 29.94	В
ATOM	1694	CD	ARG		34	51.664	-1.888	6.541	1.00 32.95	B B
MOTA	1695	NE	ARG		34 34	51.897 51.392	-1.875 -0.973	5.101 4.267	1.00 35.17 1.00 37.51	B
MOTA MOTA	1696 1697	CZ NH1	ARG ARG		34 34	50.622	0.003	4.729	1.00 37.31	В
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ATOM	1698	NH2	ARG	В	34	51.642	-1.058	2.967	1.00 36.90	В
ATOM	1699	С		В	34	49.587	-6.218	6.498	1.00 26.48	В
ATOM	1700	0	ARG	В	34	48.740	-5.639	5.825	1.00 27.17	В
ATOM	1701	N	GLU	В	35	49.647	-7.534	6.602	1.00 25.66	В
ATOM	1702	CA	GLU	В	35	48.746	-8.394	5.867	1.00 26.99	В
ATOM	1703	CB	GLU	В	35	49.570	-9.483	5.175	1.00 31.53	В
ATOM	1704	CG	GLU	В	35	48.814	-10.396	4.235	1.00 36.29	В
ATOM	1705	CD	GLU	В	35	49.695	-11.530	3.731	1.00 40.61	В
ATOM	1706	OE1	GLU	В	35	50.825	-11.240	3.276	1.00 45.20	В
ATOM	1707	OE2	GLU	В	35	49.266	-12.705	3.791	1.00 41.13	В
ATOM	1708	C	GLU	В	35	47.699	-9.031	6.764	1.00 25.09	В
ATOM	1709	0			35	48.028	-9.807	7.663	1.00 23.31	В
ATOM	1710	N	GLU		36	46.439	-8.689	6.522	1.00 24.53	В
ATOM	1711	CA	GLU		36	45.332	-9.263	7.275	1.00 25.73	В
ATOM	1712	CB	GLU		36	44.023	-8.519	6.958	1.00 26.62	В
ATOM	1713	CG	GLU		36	42.783	-9.095	7.636	1.00 28.26	В
ATOM	1714	CD	GLU		36	41.545	-8.232	7.442	1.00 31.08	В
ATOM	1715	OE1	GLU		36	41.420	-7.590	6.377	1.00 32.56	В
ATOM	1716	OE2	GLU		36	40.685	-8.206	8.349	1.00 32.83	В
ATOM	1717	C	GLU		36	45.238	-10.717	6.822	1.00 24.67	В
ATOM	1718	0			36	45.141	-10.992	5.626	1.00 23.91	В
ATOM	1719	N		В	37	45.282	-11.647	7.771	1.00 26.11	В
ATOM	1720	CA		В	37	45.219	-13.067	7.433	1.00 27.80	В
ATOM	1721	CB		В	37	46.444	-13.822	8.013	1.00 27.27	В
ATOM	1722	CG2	ILE		37	47.728		7.516	1.00 27.41	В
ATOM	1723	CG1	ILE		37		-13.767	9.537	1.00 29.35	В
ATOM	1724	CD1	ILE		37		-14.509	10.175	1.00 30.27	В
ATOM	1725	C	ILE		37		-13.750	7.879	1.00 27.86	В
ATOM	1726	0	ILE		37		-14.674	7.221	1.00 28.29	В
ATOM	1727	N	VAL		38		-13.296	8.989	1.00 28.78	В
ATOM	1728	CA	VAL		38			9.487	1.00 29.29	В
ATOM	1729	CB	VAL		38		-14.751	10.741	1.00 30.18	В
ATOM	1730	CG1			38		-15.452	11.071	1.00 33.17	В
ATOM	1731	CG2			38		-15.764	10.520	1.00 31.09	В
ATOM	1732	C	VAL		38		-12.745	9.882	1.00 28.75	В
ATOM	1733	0	VAL		38		-11.758	10.480	1.00 29.70	В
ATOM	1734	N	ARG		39		-12.911	9.581	1.00 27.05	В
ATOM	1735	CA	ARG		39		-11.890	9.892	1.00 25.46	В
ATOM	1736	CB	ARG		39		-11.064		1.00 27.23	В
ATOM	1737	CG	ARG		39		-10.011	8.765	1.00 30.84	В
ATOM	1738	CD	ARG		39	37.111			1.00 29.34	В
ATOM	1739	NE	ARG		39	38.218		6.673	1.00 30.83	В
ATOM	1740	CZ	ARG		39	38.116			1.00 31.23	В
ATOM	1741	NH1	ARG		39	36.951			1.00 31.08	В
ATOM	1742	NH2			39	39.178		4.883	1.00 30.81	В
ATOM	1742	C	ARG		39		-12.476	10.381	1.00 25.41	В
ATOM	1744	0	ARG		39			9.996	1.00 25.06	В
ATOM	1745	N	PHE		40		-11.742	11.252	1.00 23.72	В
ATOM	1745	CA	PHE		40		-12.164	11.696	1.00 24.04	В
ATOM	1747	CB	PHE		40		-12.554	13.171	1.00 22.69	В
ATOM	1748	CG	PHE		40		-13.036		1.00 20.75	B
ATOM	1749	CD1		В	40		-14.370	13.413	1.00 21.07	В
ATOM	1750	CD2		В	40		-12.135	14.003	1.00 21.00	В
ATOM	1751	CE1		В	40	32.475		13.670	1.00 20.86	В
ATOM	1752	CE2	PHE	В	40		-12.553	14.261	1.00 19.95	В
ATOM	1753	CZ	PHE	B	40	31.517		14.092	1.00 19.78	B
ATOM	1754	C	PHE	В	40	34.662		11.474	1.00 24.27	В
ATOM	1755	0	PHE	В	40	34.755		12.183	1.00 22.94	В
ATOM	1756	N	ASP	В	41	33.800		10.471	1.00 24.75	В
MOTA	1757	CA	ASP	B	41	32.857		10.101	1.00 24.98	В
ATOM	1758	CB	ASP	В	41	32.863		8.578	1.00 25.64	В
MOTA	1759	CG	ASP	В	41	32.162		8.116	1.00 27.70	В
ATOM	1760	OD1		B	41	31.163		8.749	1.00 26.21	В
MOTA	1761	OD1		В	41	32.607		7.102	1.00 30.42	B
ATOM	1761	C	ASP		41	31.477		10.560	1.00 24.50	В
ATOM	1762	0	ASP	В	41	31.011		10.151	1.00 24.95	В
ATOM	1764	N	SER		42	30.822		11.404	1.00 24.16	В
ATOM	1765	CA	SER		42		-10.096	11.882	1.00 26.13	В
ATOM	1766	CB	SER		42	29.013		12.972	1.00 24.53	В
ATOM	1767	OG	SER		42	28.932		12.497	1.00 23.39	В
ATOM	1768	G	SER		42	28.497		10.729	1.00 27.68	В
ATOM	1769	0	SER		42		-10.833	10.818	1.00 27.31	В
ATOM	1770	N	ASP		43	28.789		9.654	1.00 28.17	В
ATOM	1771	CA	ASP		43	27.924		8.477	1.00 29.40	В
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ATOM	1772	CB	ASP	В	43	28.332	-8.298	7.508	1.00 29.57	В
ATOM	1773	CG	ASP	В	43	27.587	-7.006	7.766	1.00 32.71	В
ATOM	1774	OD1	ASP	В	43	26.999	-6.868	8.862	1.00 33.94	В
ATOM	1775	OD2	ASP	В	43	27.593	-6.120	6.881	1.00 33.98	В
ATOM	1776	C	ASP	В	43	28.036	-10.762	7.782	1.00 29.46	В
ATOM	1777	0	ASP	B	43	27.162	-11.150	7.009	1.00 30.77	В
MOTA	1778	N	VAL	В	44	29.123	-11.471	8.068	1.00 27.98	В
ATOM	1779	CA	VAL	В	44	29.365	-12.780	7.486	1.00 27.16	В
ATOM	1780	CB	VAL	В	44	30.846	-12.939	7.075	1.00 27.32	В
ATOM	1781	CG1	VAL	В	44	31.083	-14.323	6.488	1.00 24.09	В
MOTA	1782	CG2	VAL	В	44	31.218	-11.857	6.073	1.00 24.66	В
ATOM	1783	C	VAL		44	28.990	-13.867	8.490	1.00 28.43	В
ATOM	1784	0	VAL	В	44	28.558	-14.948	8.108	1.00 29.45	В
ATOM	1785	N	GLY		45	29.177	-13.590	9.774	1.00 28.05	В
ATOM	1786	CA	GLY		45	28.794	-14.561	10.780	1.00 28.67	В
ATOM	1787	C	GLY		45	29.758	-15.679	11.125	1.00 28.25	В
ATOM	1788	0	GLY	В	45	29.458	-16.486	12.002	1.00 29.67	В
ATOM	1789	N	GLU	_	46	30.895	-15.755	10.443	1.00 27.03	В
ATOM	1790	CA	GLU		46	31.873	-16.787	10.757	1.00 29.26	В
ATOM	1791	CB		В	46	31.571	-18.087	10.000	1.00 32.16	В
ATOM	1792	CG	GLU	В	46	32.039	-18.121	8.554	1.00 37.36	В
ATOM	1793	CD	GLU		46	31.752	-19.458	7.885	1.00 41.59	В
ATOM	1794	OE1	GLU		46		-20.505	8.433	1.00 43.30	В
ATOM	1795	OE2	GLU		46	31.116	-19.463	6.810	1.00 43.54	В
ATOM	1796	C	GLU		46	33.272	-16.295	10.413	1.00 29.29	В
ATOM	1797	0	GLU	В	46		-15.288	9.722	1.00 30.45	В
ATOM	1798	N		В	47		-17.005	10.904	1.00 28.00	В
ATOM	1799	CA	PHE	В	47		-16.650	10.651	1.00 28.10	В
ATOM	1800	CB	PHE		47		-17.445	11.566	1.00 28.74	В
ATOM	1801	CG	PHE	В	47	36.487		13.016	1.00 30.23	В
ATOM	1802	CD1		В	47	37.248		13.535	1.00 28.96	В
ATOM	1803	CD2		В	47	35.636	-17.768	13.870	1.00 30.80	В
ATOM	1804	CE1		В	47		-15.683	14.888	1.00 31.59	В
ATOM	1805	CE2	PHE	В	47		-17.435	15.229	1.00 31.97	В
ATOM	1806	CZ	PHE	В	47	36.311		15.737	1.00 30.36	В
ATOM	1807	C	PHE	В	47		-16.948	9.211	1.00 28.71	В
ATOM	1808	0	PHE	В	47	35.576	-17.937	8.640	1.00 28.03	В
ATOM	1809	N	ARG		48	36.872	-16.091	8.637	1.00 27.96	В
ATOM	1810	CA	ARG		48	37,327		7.261	1.00 26.41	В
ATOM	1811	CB	ARG		48	36.513		6.326	1.00 26.57	В
	1812	CG	ARG		48	35.068		6.108	1.00 26.19	В
ATOM	1813	CD	ARG		48		-17.079	5.352	1.00 24.98	В
ATOM	1814	NE	ARG		48	33.579		5.146	1.00 26.01	В
ATOM		CZ	ARG		48	32.755		4.294	1.00 26.84	В
ATOM	1815	NH1			48	33.181		3.554	1.00 26.92	В
MOTA	1816		•		48	31.492		4.204	1.00 30.22	В
MOTA	1817	NH2	ARG		48	38.799		7.140	1.00 26.95	B
MOTA	1818	C	ARG		48		-14.878	7.737	1.00 24.36	B
ATOM	1819	0	ALA		49	39.542		6.373	1.00 24.93	В
ATOM	1820	N			49		-16.349	6.143	1.00 26.58	В
ATOM	1821	CA	ALA		49		-17.619	5.792	1.00 27.05	В
ATOM	1822	CB	ALA		49 49		-15.397	4.956	1.00 26.47	В
ATOM	1823	C	ALA ALA		49	_	-15.635	3.983	1.00 26.12	В
MOTA	1824	O N	VAL		4 0		-14.302	5.044	1.00 27.06	В
MOTA	1825	CA	VAL		50		-13.357	3.936	1.00 26.50	В
ATOM	1826		VAL		50		-11.876	4.439	1.00 27.14	В
MOTA	1827	CB CG1			50		-11.827	5.846	1.00 29.89	В
ATOM	1828	CG2			50		-11.020	3.501	1.00 27.33	В
ATOM	1829	C	VAL		50		-13.742	3.037	1.00 26.58	В
ATOM	1830	0	VAL		50		-13.390	1.860	1.00 27.84	В
MOTA	1831		THR		51		-14.489	3.598	1.00 26.61	В
MOTA	1832	N			51		-15.011	2.846	1.00 28.59	В
MOTA	1833	CA	THR		51		-14.193	3.056	1.00 28.25	В
ATOM	1834	CB	THR				-14.464	4.356	1.00 28.56	В
ATOM	1835	OG1			51 51		-12.699	2.899	1.00 27.40	В
MOTA	1836	CG2			51 51		-12.699	3.344	1.00 27.40	В
MOTA	1837	C	THR		51 51		7 -16.435	4.418	1.00 20.25	В
MOTA	1838	O	THR		51 52			2.575	1.00 30.18	В
ATOM	1839	N	LEU				-17.217 -18.596	2.575	1.00 30.34	В
ATOM	1840	CA	LEU		52 52			1.963	1.00 32.19	В
ATOM	1841	CB	LEU		52 52		7 -19.237	0.624	1.00 36.90	В
ATOM	1842	CG	LEU		52 52		-19.724	-0.216	1.00 35.68	В
MOTA	1843	CD1			52 52		-20.306 -20.775	0.861	1.00 35.34	В
ATOM	1844	CD2			52 52		2 -18.724	4.359	1.00 33.54	В
MOTA	1845	С	LEU	, 5	JA	∓0. 07∠	-10./24	4.33 3	<u> </u>	.

ATOM	1846	0	LEU	B	52	46.570 -19.	656	5.097	1.00 31.50	В
ATOM	1847	N	LEU	В	53	47.753 -17.	786	4.723	1.00 31.09	В
ATOM	1848	CA	LEU	В	53	48.388 -17.	815	6.029	1.00 30.93	В
ATOM	1849	CB		В	53	49.160 -16.		6.246	1.00 31.99	В
		CG		В	53	50.338 -16.		7.221	1.00 35.20	В
ATOM	1850									
ATOM	1851	CD1	LEU		53	51.364 -17.		6.763	1.00 35.92	В
ATOM	1852	CD2	LEU	В	53	50.975 -15.	148	7.284	1.00 34.96	B
ATOM	1853	C	LEU	В	53	47.377 -18.	017	7.160	1.00 29.90	В
ATOM	1854	0	LEU	В	53	47.663 -18.	709	8.138	1.00 30.68	В
ATOM	1855	N	GLY	R	54	46.192 -17.	430	7.015	1.00 28.63	В
		CA	GLY		54	45.181 -17.		8.057	1.00 29.75	В
ATOM	1856							7.901		В
MOTA	1857	C	GLY		54	44.140 -18.				
ATOM	1858	0	GLY	В	54	43.146 -18.	664	8.630	1.00 28.02	В
ATOM	1859	N	LEU	В	55	44.364 -19.	547	6.964	1.00 30.54	В
MOTA	1860	CA	LEU	В	55	43.417 -20.	630	6.732	1.00 32.59	В
ATOM	1861	CB	LEU	В	55	43.765 -21.	344	5.422	1.00 35.94	В
ATOM	1862	CG		В	55	42.776 -22.	383	4.889	1.00 38.88	В
				В	55	41.355 -21.		4.927	1.00 38.23	B
ATOM	1863	CD1								
ATOM	1864	CD2		В	55	43.173 -22.		3.467	1.00 39.03	B
ATOM	1865	C	LEU	В	55	43.330 -21.	631	7.892	1.00 32.20	В
ATOM	1866	0	LEU	В	55	42.235 -22.	.026	8.291	1.00 33.32	В
ATOM	1867	N	PRO	В	56	44.478 -22.	058	8.447	1.00 31.03	В
ATOM	1868	CD	PRO	В	56	45.862 -21.	.802	8.009	1.00 30.17	В
ATOM	1869	CA		В	56	44.451 -23.		9.561	1.00 30.23	В
						45.925 -23.		9.931	1.00 30.27	В
ATOM	1870	CB	PRO		56					В
ATOM	1871	CG	PRO		56	46.609 -22		8.610	1.00 28.92	
MOTA	1872	C	PRO	В	56	43.613 -22	.525	10.740	1.00 31.42	B
ATOM	1873	0	PRO	В	56	42.730 -23	.237	11.222	1.00 33.17	В
ATOM	1874	N	ALA	В	57	43.893 -21	305	11.196	1.00 30.04	В
ATOM	1875	CA	ALA	В	57	43.181 -20	719	12.322	1.00 28.60	В
ATOM	1876	CB	ALA		57	43.818 -19	.389	12.697	1.00 26.81	В
					57	41.695 -20		12.021	1.00 29.08	В
ATOM	1877	C	ALA							В
MOTA	1878	0	ALA		57		. 737	12.887	1.00 28.22	
MOTA	1879	N	ALA	В	58	41.385 -20	.135	10.791	1.00 28.84	В
ATOM	1880	CA	ALA	В	58	40.002 -19	.922	10.386	1.00 31.06	В
ATOM	1881	CB	ALA	В	58	39.955 -19	.426	8.947	1.00 29.79	В
ATOM	1882	C	ALA	В	58	39.169 -21	.199	10.529	1.00 32.38	В
ATOM	1883	0	ALA		58		.197	11.170	1.00 31.57	В
					59		.285	9.929	1.00 33.50	В
MOTA	1884	N	GLU							
ATOM	1885	CA	GLU		59	38.949 -23		9.993	1.00 33.91	В
MOTA	1886	CB	GLU	B	59	39.706 -24		9.195	1.00 35.67	В
MOTA	1887	CG	$\mathtt{GL}\mathtt{U}$	В	59	39.619 -24	.457	7.696	1.00 39.73	В
ATOM	1888	CD	GLU	В	59	40.327 -25	.583	6.957	1.00 43.58	В
ATOM	1889	OE1	GLU	В	59	41.561 -25	.715	7.119	1.00 44.52	В
ATOM	1890	OE2	GLU	В	59	39.648 -26	.337	6.222	1.00 44.30	В
		C	GLU		59	38.771 -24		11.425	1.00 33.56	В
ATOM	1891							11.790	1.00 34.40	В
ATOM	1892	0	GLU		59	37.708 -24				
MOTA	1893	N	TYR		60	39.815 -23		12.233	1.00 31.99	B
ATOM	1894	CA	TYR	B	60	39.754 -24	.369	13.611	1.00 31.01	В
MOTA	1895	CB	TYR	В	60	41.112 -24	.202	14.292	1.00 31.13	B
ATOM	1896	CG	TYR	В	60	41.051 -24	.548	15.750	1.00 30.99	В
ATOM	1897	CD1	TYR	В	60	40.919 -25	.871	16.162	1.00 32.55	В
ATOM	1898		TYR		60	40.770 -26		17.508	1.00 35.39	В
					60	41.039 -23		16.716	1.00 32.67	В
ATOM	1899	CD2								
MOTA	1900	CE2			60	40.890 -23		18.064		В
ATOM	1901	CZ	TYR	В	60	40.756 -25		18.455	1.00 36.91	B -
MOTA	1902	OH	TYR	B	60	40.606 -25	.483	19.791	1.00 40.06	В
ATOM	1903	C	TYR	\mathbf{B}	60	38.695 -23	.631	14.426	1.00 31.72	В
MOTA	1904	0	TYR	В	60	37.840 -24	.258	15.050	1.00 31.72	В
ATOM	1905	N	TRP		61	38.752 -22	.303	14.428	1.00 30.37	В
			TRP		61	37.790 -21		15.194	1.00 31.57	В
ATOM	1906	CA							1.00 32.14	В
MOTA	1907	CB	TRP		61	38.129 -20		15.140		
MOTA	1908	CG	TRP	В	61	39.430 -19		15.824	1.00 33.73	В
MOTA	1909	CD2	TRP	B	61	40.359 -18		15.429	1.00 35.16	В
ATOM	1910	CE2	TRP	В	61	41.418 -18	.662	16.362	1.00 35.99	В
MOTA	1911	CE3	TRP	B	61	40.397 -17	.719	14.378	1.00 38.30	В
MOTA	1912	CD1			61	39.949 -20		16.949	1.00 33.63	В
ATOM	1913		TRP		61	41.142 -19		17.278	1.00 33.97	В
					61	42.512 -17		16.277	1.00 38.13	В
ATOM	1914	CZ2								В
MOTA	1915	CZ3			61	41.487 -16		14.293	1.00 39.26	
MOTA	1916	CH2			61	42.527 -16		15.240	1.00 38.22	В
ATOM	1917	C	TRP	В	61	36.349 -21		14.739	1.00 31.22	B
ATOM	1918	0	TRP	В	61	35.436 -21	.758	15.559	1.00 29.98	B
ATOM	1919	N	ASN	В	62	36.137 -21	.955	13.440	1.00 31.63	В
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MOTA	1920	CA	ASN	В	62	34.781 -22.191 12.950 1.00 32.57	В
ATOM	1921	СВ	ASN	В	62	34.701 -22.021 11.434 1.00 30.37	В
ATOM	1922	CG	ASN	В	62	34.575 -20.574 11.025 1.00 29.69	В
ATOM	1923	OD1	ASN	В	62	33.889 -19.794 11.680 1.00 29.42	В
ATOM	1924	ND2	ASN	В	62	35.222 -20.209 9.926 1.00 31.50	В
ATOM	1925	C	ASN		62	34.238 -23.561 13.339 1.00 32.87	В
ATOM	1926	0	ASN		62	33.028 -23.789 13.292 1.00 34.70	
ATOM	1927	N	SER		63	35.128 -24.469 13.725 1.00 32.43	
	1928	CA	SER		63	34.705 -25.797 14.140 1.00 32.38	
ATOM						35.818 -26.819 13.879 1.00 32.20	
ATOM	1929	CB	SER		63		
MOTA	1930	OG	SER		63	36.905 -26.626 14.760 1.00 33.33	
MOTA	1931	C	SER		63	34.348 -25.768 15.630 1.00 32.14	
MOTA	1932	0	SER		63	33.677 -26.667 16.138 1.00 32.86	
MOTA	1933	N	GLN	B	64	34.794 -24.724 16.325 1.00 31.10	
ATOM	1934	CA	GLN	В	64	34.513 -24.569 17.752 1.00 30.99	
MOTA	1935	CB	GLN	B	64	35.661 -23.837 18.446 1.00 32.54	
ATOM	1936	CG	GLN	В	64	36.988 -24.557 18.383 1.00 34.49	B
MOTA	1937	CD	GLN	В	64	36.870 -25.998 18.810 1.00 38.20) B
ATOM	1938	OE1	GLN	В	64	36.629 -26.884 17.984 1.00 40.82	B B
ATOM	1939	NE2	GLN	В	64	37.022 -26.245 20.108 1.00 38.34	B
ATOM	1940	C	GLN	В	64	33.226 -23.775 17.944 1.00 29.88	B B
ATOM	1941	0		В	64	33.252 -22.549 18.064 1.00 29.28	B
MOTA	1942	N	LYS		65	32.101 -24.476 17.979 1.00 28.74	В
ATOM	1943	CA		В	65	30.815 -23.812 18.123 1.00 29.18	
		CB	LYS		65	29.688 -24.851 18.132 1.00 30.63	
ATOM	1944					29.575 -25.612 16.812 1.00 32.20	
ATOM	1945	CG	LYS		65		
ATOM	1946	CD	LYS		65		
ATOM	1947	CE	LYS		65	29.688 -25.327 14.284 1.00 37.24	
MOTA	1948	NZ	LYS		65	29.430 -24.427 13.109 1.00 37.89	
ATOM	1949	С	LYS	В	65	30.745 -22.919 19.352 1.00 28.19	
MOTA	1950	0	LYS	В	65	30.075 -21.891 19.333 1.00 28.16	
MOTA	1951	N	ASP	В	66	31.440 -23.304 20.417 1.00 27.58	
ATOM	1952	CA	ASP	B	66	31.460 -22.504 21.636 1.00 27.43	L B
ATOM	1953	CB	ASP	${\tt B}$	66	32.283 -23.208 22.727 1.00 28.49	5 B
MOTA	1954	CG	ASP	В	66	33.559 -23.847 22.184 1.00 32.24	a B
ATOM	1955	QD1	ASP	В	66	33.478 -24.591 21.183 1.00 33.1	7 B
ATOM	1956	OD2		В	66	34.642 -23.623 22.765 1.00 33.25	5 B
ATOM	1957	C		В	66	32.050 -21.131 21.316 1.00 26.63	B B
ATOM	1958	0		В	66	31.468 -20.102 21.662 1.00 24.32	
ATOM	1959	N	ILE	В	67	33.198 -21.116 20.640 1.00 26.13	
				В	67	33.840 -19.855 20.273 1.00 26.42	
ATOM	1960	CA			67	35.206 -20.088 19.613 1.00 28.29	
ATOM	1961	CB	ILE				
MOTA	1962	CG2	ILE		67 67		
ATOM	1963	CG1		В	67		
ATOM	1964	CD1			67	36.319 -20.321 21.906 1.00 32.60	
MOTA	1965	C	ILE	В	67	32.968 -19.061 19.300 1.00 26.30	
MOTA	1966	0	ILE	B	67	32.747 -17.869 19.491 1.00 25.3	
ATOM	1967	N	LEU	В	68	32.472 -19.730 18.261 1.00 26.13	
ATOM	1968	CA	LEU	B	68	31.617 -19.086 17.267 1.00 26.6	
MOTA	1969	CB	LEU	В	68	31.132 -20.102 16.235 1.00 27.63	
ATOM	1970	CG	LEU	B	68	31.807 -20.171 14.872 1.00 30.13	
ATOM	1971	CD1	LEU	В	68	31.081 -21.216 14.031 1.00 33.0	
MOTA	1972	CD2	LEU	\mathbb{B}	68	31.766 -18.812 14.190 1.00 30.0	1 B
MOTA	1973	C	LEU	В	68	30.394 -18.415 17.878 1.00 26.8	1 B
ATOM	1974	0	LEU	В	68	30.067 -17.280 17.541 1.00 26.1	9 B
MOTA	1975	N	GLU	В	69	29.706 -19.135 18.756 1.00 28.8	7 B
ATOM	1976	CA	GLU	В	69	28.509 -18.614 19.404 1.00 31.5	5 B
ATOM	1977	CB	GLU		69	27.945 -19.654 20.382 1.00 35.7	5 B
MOTA	1978	CG	GLU		69	27.304 -20.862 19.695 1.00 43.7	1 B
ATOM	1979	CD	GLU		69	26.883 -21.954 20.673 1.00 47.9	2 В
ATOM	1980	OE1			69	27.756 -22.454 21.418 1.00 49.2	
	1981	OE2			69	25.683 -22.316 20.694 1.00 50.4	
MOTA		C	GLU		69	28.773 -17.295 20.130 1.00 29.8	
ATOM	1982						
ATOM	1983	O NT	GLU		69 70	27.986 -16.356	
ATOM	1984	N	ARG		70 70		
ATOM	1985	CA	ARG		70 70		
MOTA	1986	CB	ARG		70	31.347 -16.315 22.606 1.00 28.9	
ATOM	1987	CG	ARG		70	30.982 -17.344 23.673 1.00 30.5	
MOTA	1988	CD	ARG		70	32.251 -17.810 24.371 1.00 32.3	
MOTA	1989	NE	ARG		70	32.040 -19.037 25.117 1.00 34.8	
ATOM	1990	CZ	ARG		70	32.946 -19.997 25.232 1.00 34.9	
ATOM	1991	NH1	ARG	B	70	34.131 -19.875 24.647 1.00 35.0	
MOTA	1992	NH2	ARG	В	70	32.662 -21.083 25.930 1.00 39.4	
MOTA	1993	C	ARG	В	70	30.691 -14.888 20.682 1.00 26.7	7 B

ATOM	1994	0	ARG B	70	30.412	-13.725	20.951	1.00 26.95	В
ATOM	1995	N	LYS B	71	31.395	-15.235	19.608	1.00 25.97	В
ATOM	1996	CA	LYS B	71	31.885	-14.236	18.670	1.00 25.98	В
•		CB	LYS B	71		-14.877	17.652	1.00 27.62	В
ATOM	1997					-13.873	16.924	1.00 29.24	В
ATOM	1998	CG	LYS B	71					
MOTA	1999	CD	LYS B	71		-13.137	17.909	1.00 32.14	B
ATOM	2000	CE	LYS B	71	35.430	-12.035	17.236	1.00 33.13	В
ATOM	2001	NZ	LYS B	71	36.093	-11.164	18.245	1.00 34.18	В
ATOM	2002	С	LYS B	71	30.710	-13.591	17.952	1.00 25.22	В
						-12.395	17.671	1.00 24.39	В
MOTA	2003	0	LYS B	71					
MOTA	2004	N	ARG B	72	_ · · · ·	-14.399	17.657	1.00 25.08	В
MOTA	2005	CA	ARG B	72	28.500	-13.922	16.989	1.00 26.32	В
ATOM	2006	CB	ARG B	72	27.628	-15.101	16.561	1.00 28.02	В
ATOM	2007	CG	ARG B	72	28.116	-15.830	15.340	1.00 28.10	В
ATOM	2008	CD	ARG B	72		-17.013	15.083	1.00 32.02	В
						-17.583	13.766	1.00 36.46	В
MOTA	2009	NE	ARG B	72					
MOTA	2010	CZ	ARG B	72		-18.779	13.389	1.00 38.62	B
MOTA	2011	NHl	ARG B	72	26.324	-19.538	14.238	1.00 37.88	B
ATOM	2012	NH2	ARG B	72	27.270	-19.212	12.163	1.00 38.55	В
ATOM	2013	С	ARG B	72	27.687	-13.017	17.898	1.00 24.31	В
			ARG B			-12.326	17.439	1.00 24.84	В
ATOM	2014	0						1.00 26.18	В
ATOM	2015	N	ALA B		27.990	-13.028	19.189		
MOTA	2016	CA	ALA B	73	27.267	-12.185	20.140	1.00 28.18	B
ATOM	2017	CB	ALA B	73	26.973	-12.974	21.418	1.00 28.97	В
ATOM	2018	C	ALA B	73	28.056	-10.916	20.472	1.00 28.97	В
ATOM	2019	Ō	ALA B		27.528	-9.977	21.066	1.00 30.50	В
					29.320	-10.882	20.070	1.00 29.65	В
ATOM	2020	N	ALA B					1.00 30.77	В
ATOM	2021	CA	ALA B		30.170	-9.732	20.347		
MOTA	2022	CB	ALA B	74	31.558	-9.966	19.764	1.00 30.77	В
ATOM	2023	С	ALA B	74	29.594	-8.414	19.827	1.00 31.78	В
ATOM	2024	0	ALA B	74	29.789	-7.359	20.438	1.00 32.74	В
ATOM	2025	N	VAL B		28.886	-8.465	18.704	1.00 31.60	В
					28.308	-7.248	18.145	1.00 32.38	В
MOTA	2026	CA	VAL B						В
MOTA	2027	CB	VAL B	75	27.397	-7.539	16.929	1.00 30.51	
MOTA	2028	CG1	VAL B	75	27.291	-6.295	16.062	1.00 31.44	В
ATOM	2029	CG2	VAL B	75	27.931	-8.696	16.137	1.00 33.08	В
ATOM	2030	C	VAL B	75	27.465	-6.529	19.201	1.00 33.07	В
		0	VAL B		27.402	-5.302	19.218	1.00 33.54	В
ATOM	2031						20.065	1.00 34.70	В
MOTA	2032	N	ASP B		26.811	-7.302			
ATOM	2033	CA	ASP B	76	25.971	-6.748	21.130	1.00 36.27	B -
ATOM	2034	CB	ASP B	76	24.780	-7.670	21.420	1.00 38.57	В
ATOM	2035	CG	ASP B	76	23.889	-7.881	20.215	1.00 41.48	В
ATOM	2036	OD1	ASP B	76	23.335	-6.887	19.694	1.00 43.46	В
					23.739	-9.048	19.792	1.00 43.76	В
ATOM	2037	OD2					22.411	1.00 35.56	В
MOTA	2038	C	ASP B		26.780	-6.600			
MOTA	2039	0	ASP E	76	26.731	-5.569	23.081	1.00 34.13	B -
ATOM	2040	N	ARG E	3 77	27.508	-7.661	22.744	1.00 35.22	В
ATOM	2041	CA	ARG E	3 77	28.343	-7.708	23.937	1.00 34.49	В
ATOM	2042	CB	ARG E	3 77	29.071	-9.052	23.991	1.00 37.16	B
	2043	CG	ARG E		29.841	-9.328	25.271	1.00 40.90	В
MOTA							25.102	1.00 43.79	В
ATOM	2044	CD	ARG E			-10.553			В
MOTA	2045	NE	ARG E		30.004		24.665	1.00 48.65	
MOTA	2046	CZ	ARG E	3 77	29.103	-12.385	25.406	1.00 51.36	В
MOTA	2047	NH1	. ARG E	3 77	28.816	-11.949	26.626	1.00 52.34	В
MOTA	2048	NH2	ARG E	3 77	28.499	-13.470	24.935	1.00 50.76	В
ATOM	2049	C	ARG E		29.362	-6.576	23.927	1.00 32.18	В
					29.499		24.896	1.00 32.49	В
MOTA	2050	0	ARG E					1.00 30.66	В
MOTA	2051	N	VAL E		30.073		22.818		
ATOM	2052	CA	VAL E	3 78	31.086	-5.414	22.707	1.00 29.00	В
MOTA	2053	CB	VAL E	3 78	32.276	-5.917	21.867	1.00 27.82	В
ATOM	2054	CG1	VAL E	3 78	33.327	-4.815	21.740	1.00 25.08	В
ATOM	2055	CG2			32.870		22.504	1.00 23.27	В
							22.113	1.00 29.33	В
MOTA	2056	C	VAL I		30.594				В
MOTA	2057	0	VAL I		30.435		22.831	1.00 29.83	
MOTA	2058	N	CYS I	3 79	30.354	-4.091	20.804	1.00 28.42	В
ATOM	2059	CA	CYS I	B 79	29.927	-2.891	20.083	1.00 29.14	В
ATOM	2060	C	CYS I	B 79	28.724	-2.107	20.629	1.00 28.59	В
ATOM	2061	0		B 79	28.883		21.062	1.00 26.06	В
					29.675		18.604	1.00 29.19	В
MOTA	2062	CB	CYS I						В
ATOM	2063	SG	CYS I		31.052		17.680	1.00 31.71	
MOTA	2064	N	ARG I	B 80	27.527	-2.693	20.586	1.00 28.34	В
ATOM	2065	CA	ARG	B 80	26.347	-1.980	21.071	1.00 30.77	В
ATOM	2066	CB	ARG 1	B 80	25.079	-2.828	20.915	1.00 32.82	В
	2067	CG	ARG :		24.612		19.474	1.00 35.65	В
MOTA	2007				محدث و بر بد		,,,		

ATOM	2068	CD	ARG	R	80	23.120	-3.273	19.387	1.00 36.01	В
ATOM	2069	NE		В	80	22.649	-3.243	18.005	1.00 35.49	B
					80	22.913	-4.188	17.108	1.00 33.19	B
ATOM	2070	CZ	ARG							В
ATOM	2071	NH1		B	80	23.640	-5.242	17.449	1.00 40.57	
MOTA	2072	NH2	ARG	В	80	22.467	-4.075	15.864	1.00 38.86	B
MOTA	2073	C	ARG	В	80	26.507	-1.552	22.524	1.00 31.24	В
ATOM	2074	0	ARG	В	80	25.975	-0.525	22.944	1.00 32.07	В
ATOM	2075	N	HIS	В	81	27.257	-2.337	23.283	1.00 31.40	В
ATOM	2076	CA	HIS	В	81	27.492	-2.028	24.683	1.00 32.20	В
ATOM	2077	CB		В	81	28.220	-3.185	25.366	1.00 33.00	В
ATOM	2078	CG		В	81	28.595	-2.899	26.787	1.00 37.24	В
	2079	CD2		В	81	29.764	-2.490	27.335	1.00 38.05	В
ATOM						27.692	-2.981	27.826	1.00 39.11	В
ATOM	2080	ND1		B	81					
ATOM	2081	CE1		В	81	28.290	-2.635	28.952	1.00 40.49	В
MOTA	2082	NE2	HIS	В	81	29.548	-2.332	28.682	1.00 39.16	B
MOTA	2083	C	HIS	В	81	28.326	-0.762	24.831	1.00 30.87	В
ATOM	2084	0	HIS	B	81	27.906	0.206	25.470	1.00 31.38	В
MOTA	2085	N	ASN	В	82	29.511	-0.770	24.233	1.00 29.77	, B
ATOM	2086	CA	ASN	В	82	30.403	0.375	24.332	1.00 28.02	В
ATOM	2087	CB	ASN	В	82	31.755	0.056	23.683	1.00 26.64	В
ATOM	2088	ÇG	ASN		82	32.470	-1.092	24.373	1.00 25.02	В
	2089	OD1	ASN		82	32.305	-1.305	25.572	1.00 24.06	В
ATOM					82	33.278	-1.829	23.619	1.00 26.38	В
MOTA	2090	ND2		B						В
MOTA	2091	C		В	82	29.819	1.648	23.741		
MOTA	2092	0	ASN		82	30.163	2.747	24.174	1.00 25.71	В
MOTA	2093	N	TYR	В	83	28.930	1.512	22.765	1.00 25.90	В
MOTA	2094	CA	TYR	В	83	28.324	2.693	22.156	1.00 25.91	В
MOTA	2095	CB	TYR	B	83	27.462	2.297	20.946	1.00 25.69	В
ATOM	2096	CG	TYR	В	83	27.102	3.462	20.056	1.00 25.95	В
ATOM	2097	CD1	TYR	В	83	26.022	4.294	20.353	1.00 27.11	В
ATOM	2098	CEI			83	25.712	5.403	19.545	1.00 25.98	В
	2099	CD2			83	27.865	3.759	18.933	1.00 27.72	В
ATOM						27.567	4.862	18.121	1.00 28.05	В
ATOM	2100	CE2	TYR		83				1.00 27.73	В
ATOM	2101	CZ	TYR		83	26.493	5.680	18.434		
ATOM	2102	OH	TYR		83	26.225	6.781	17.645	1.00 27.55	В
MOTA	2103	С	TYR	В	83	27.485	3.458	23.181	1.00 25.87	B
MOTA	2104	0	TYR	\mathbb{B}	83	27.315	4.673	23.070	1.00 26.05	В
ATOM	2105	N	GLN	В	84	26.975	2.750	24.186	1.00 28.25	В
ATOM	2106	CA	GLN	В	84	26.159	3.375	25.229	1.00 30.44	B
ATOM	2107	CB	GLN		84	25.467	2.310	26.093	1.00 34.30	В
ATOM	2108	CG	GLN		84	24.595	1.343	25.301	1.00 40.52	В
ATOM	2109	CD	GLN		84	23.515	2.047	24.496	1.00 43.21	В
		OE1	GLN		84	23.023	1.516	23.499	1.00 46.12	В
ATOM	2110						3.244	24.932	1.00 45.41	В
MOTA	2111	NE2	GLN		84	23.133			1.00 29.01	В
MOTA	2112	C	GLN		84	27.030	4.254	26.111		
MOTA	2113	0	GLN		84	26.633	5.353	26.494	1.00 27.82	В
MOTA	2114	N	LEU	B	85	28.219	3.757	26.436	1.00 28.32	В
MOTA	2115	CA	LEU	В	85	29.150	4.505	27.263	1.00 28.76	В
MOTA	2116	CB	LEU	В	85	30.355	3.631	27.631	1.00 28.92	В
ATOM	2117	CG	LEU	В	85	30.065	2.226	28.184	1.00 30.98	В
ATOM	2118	CD1	LEU	В	85	31.343	1.631	28.758	1.00 30.59	В
ATOM	2119	CD2			85	29.006	2.291	29.265	1.00 31.87	В
ATOM	2120	C	LEU		85	29.609	5.719	26.461	1.00 29.95	В
ATOM	2121	0	LEU		85	29.836	6.798	27.010	1.00 30.93	В
			GLU		86	29.724	5.529	25.150	1.00 30.31	В
ATOM	2122	N					6.577	24.245	1.00 31.41	В
ATOM	2123	CA	GLU		86	30.160				В
MOTA	2124	CB	- GLU		86	30.426	5.981	22.861	1.00 32.60	
ATOM	2125	CG	GLU		86	31.741	6.420	22.236	1.00 39.25	В
MOTA	2126	CD	GLU	В	86	32.962	5.854	22.953	1.00 41.02	B
MOTA	2127	OE1	GLU	В	86	33.379	4.714	22.636	1.00 40.75	В
ATOM	2128	OE2	GLU	В	86	33.497	6.553	23.843	1.00 41.96	В
ATOM	2129	C	GLU	В	86	29.113	7.684	24.146	1.00 32.44	В
MOTA	2130	0	GLU		86	29.454	8.865	24.109	1.00 30.73	В
ATOM	2131	N	LEU		87	27.838	7.303	24.103	1.00 33.77	В
	2132	CA	LEU		87	26.755	8.282	24.015	1.00 34.65	В
ATOM						25.398	7.583	23.899	1.00 34.69	В
MOTA	2133	CB	LEU		87					В
ATOM	2134	CG	LEU		87	24.916	7.169	22.508	1.00 36.86	
ATOM	2135		. LEU		87	23.655	6.326	22.642	1.00 35.43	В
ATOM	2136	CD2	LEU	В	87	24.645	8.411	21.660	1.00 35.76	B
ATOM	2137	С	LEU	В	87	26.740	9.199	25.231	1.00 35.16	В
ATOM	2138	0	LEU	В	87	26.250	10.326	25.164	1.00 34.29	В
ATOM	2139	N	ARG	В	88	27.280	8.711	26.343	1.00 36.69	В
ATOM	2140	CA	ARG		88	27.317	9.493	27.573	1.00 37.64	В
ATOM	2141	CB	ARG		88	27.173	8.575	28.791	1.00 39.79	В
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ATOM	2142	CG	ARG	B	88	25.827	7.878	28.908	1.00 45.19	
ATOM	2143	CD	ARG	B	88	25.704	7.173	30.253	1.00 49.04	В
ATOM	2144	NE	ARG	В	88	26.657	6.074	30.388	1.00 54.57	В
										В
ATOM	2145	CZ	ARG	В	88	27.101	5.603	31.552	1.00 55.76	
MOTA	2146	NH1	ARG	В	88	26.683	6.137	32.694	1.00 55.56	В
ATOM	2147	NH2	ARG	В	88	27.963	4.595	31.574	1.00 56.11	В
ATOM	2148	C	ARG	В	88	28.601	10.299	27.714	1.00 36.93	В
ATOM	2149	0	ARG	В	88	28.702	11.160	28.589	1.00 37.24	В
		_		В	89	29.571	10.035	26.842	1.00 35.19	В
MOTA	2150	N								
ATOM	2151	CA	THR	В	89	30.860	10.712	26.914	1.00 31.71	В
ATOM	2152	CB	THR	В	89	31.916	9.767	27.529	1.00 31.61	В
								26.762	1.00 29.72	В
ATOM	2153	OG1	THR	B	89	31.980	8.554			
ATOM	2154	CG2	THR	В	89	31.557	9.436	28.963	1.00 25.87	В
ATOM	2155	C	THR	R	89	31.420	11.254	25.600	1.00 31.31	В
										В
MOTA	2156	0	THR	В	89	31.214	12.415	25.249	1.00 32.41	
ATOM	2157	N	THR	В	90	32.139	10.403	24.880	1.00 30.72	В
	2158	CA	THR	מי	90	32.766	10.786	23.623	1.00 30.43	В
ATOM										
ATOM	2159	CB	THR	В	90	33.368	9.558	22.925	1.00 30.54	В
ATOM	2160	OG1	THR	В	90	34.297	8.919	23.808	1.00 33.70	В
						34.099	9.970	21.666	1.00 31.65	В
ATOM	2161	CG2	THR	B	90					
ATOM	2162	C	THR	В	90	31.874	11.512	22.625	1.00 30.61	, B
ATOM	2163	0	THR	R	90	32.267	12.543	22.070	1.00 30.24	В
										В
ATOM	2164	N	LEU	В	91	30.683	10.977	22.385		
MOTA	2165	ÇA	LEU	В	91	29.767	11.581	21.425	1.00 31.93	В
ATOM	2166	СВ	LEU	בר	91	28.709	10.554	21.007	1.00 32.55	В
ATOM	2167	CG	LEU	В	91	29.268	9.315	20.292	1.00 33.01	В
ATOM	2168	CD1	LEU	В	91	28.201	8.233	20.205	1.00 33.73	В
		CD2		В	91	29.761	9.700	18.902	1.00 31.26	В
MOTA	2169									
MOTA	2170	C	\mathtt{LEU}	B	91	29.096	12.872	21.907	1.00 32.38	В
ATOM	2171	0	LEU	В	91	28.402	13.534	21.139	1.00 32.08	В
						29.303	13.229	23.173	1.00 32.44	В
MOTA	2172	N	GLN	В	92					
ATOM	2173	CA	${ t GLN}$	В	92	28.725	14.454	23.713	1.00 34.54	В
ATOM	2174	CB	GLN	В	92	28.138	14.217	25.110	1.00 38.48	В
								25.121	1.00 44.66	В
MOTA	2175	CG	GLN	B	92	26.836	13.419			
MOTA	2176	CD	GLN	В	92	26.233	13.291	26.516	1.00 49.27	В
ATOM	2177	OE1	GLN	Þ	92	25.239	12.588	26.712	1.00 51.65	В
										В
ATOM	2178	NE2	GLN	В	92	26.832	13.975	27.491	1.00 49.93	
MOTA	2179	C	GLN	В	92	29.779	15.557	23.777	1.00 32.86	' B
					92	29.457	16.721	24.019	1.00 32.19	В
ATOM	2180	0	GLN							
ATOM	2181	N	ARG	В	93	31.038	15.187	23.555	1.00 31.53	В
ATOM	2182	CA	ARG	B	93	32.132	16.157	23.576	1.00 29.87	В
								23.302	1.00 28.14	В
MOTA	2183	CB	ARG	В	93	33.477	15.472			
ATOM	2184	CG	ARG	B	93	34.681	16.433	23.217	1.00 23.56	В
ATOM	2185	CD	ARG	R	93	35.953	15.656	22.925	1.00 22.53	В
										В
ATOM	2186	NE	ARG	В	93	37.128	16.486	22.662		
ATOM	2187	CZ	ARG	В	93	37.769	17.205	23.581	1.00 18.66	В
ATOM	2188	NH1	ARG	Þ	93	37.352	17.214	24.843	1.00 17.45	В
										В
ATOM	2189	NH2	ARG	В	93	38.847	17.898	23.242	1.00 16.56	
MOTA	2190	C	ARG	В	93	31.921	17.245	22.535	1.00 29.02	B
	2191	0	ARG		93	31.755	16.965	21.349	1.00 29.55	В
ATOM										
MOTA	2192	N	ARG	В	94	31.933	18.490	22.987	1.00 28.71	В
MOTA	2193	CA	ARG	В	94	31.767	19.613	22.087	1.00 29.63	B
	2194	CB	ARG		94	30.299	20.046	22.041	1.00 32.44	В
MOTA										
MOTA	2195	CG	ARG	В	94	29.506	19.196	21.060	1.00 37.10	В
ATOM	2196	CD	ARG	В	94	28.016	19.414	21.124	1.00 39.80	В
					94	27.350	18.742	20.008	1.00 44.04	В
MOTA	2197	NE	ARG							
ATOM	2198	CZ	ARG	В	94	27.372	17.428	19.791	1.00 44.11	В
ATOM	2199	NH1	ARG	В	94	28.026	16.625	20.617	1.00 45.60	В
							16.916	18.739	1.00 44.45	В
ATOM	2200	NH2	ARG	В	94	26.747				
ATOM	2201	C	ARG	В	94	32.656	20.760	22.498	1.00 28.84	В
MOTA	2202	0	ARG	B	94	32.464	21.363	23.550	1.00 29.13	В
ATOM	2203	N	VAL	В	95	33.650	21.038	21.663	1.00 27.49	В
ATOM	2204	CA	VAL	В	95	34.592	22.117	21.916	1.00 26.47	В
	2205	CB	VAL		95	36.047	21.605	21.890	1.00 25.65	В
MOTA										
MOTA	2206	CG1	. VAL	В	95	37.004	22.734	22.260	1.00 22.82	В
ATOM	2207	CG2	VAL	B	95	36.202	20.423	22.849	1.00 26.01	В
							23.180	20.840	1.00 27.00	В
MOTA	2208	C	VAL		95	34.415				
ATOM	2209	0	VAL	В	95	34.721	22.945	19.665	1.00 27.00	В
ATOM	2210	N	GLU	R	96	33.912	24.340	21.253	1.00 26.94	В
									1.00 26.50	В
ATOM	2211	CA	GLU		96	33.673	25.462	20.348		
MOTA	2212	CB	GLU	В	96	33.072	26.649	21.107	1.00 29.19	В
ATOM	2213	CG	GLU		96	31.736	26.372	21.775	1.00 36.47	В
MOTA	2214	CD	GLU	В	96	31.211	27.582	22.537	1.00 40.45	В
ATOM	2215	OE1	L GLU	В	96	30.121	27.477	23.144	1.00 42.85	В
				_	-					

28.634 22.526 OE2 GLU B 31.891 1.00 40.11 В MOTA 2216 96 В GLU B 34.960 25.916 19.689 1.00 25.02 MOTA 2217 96 C GLU B 96 35.999 26.022 20.338 1.00 24.73 \mathbf{B} ATOM 2218 0 1.00 24.54 \mathbf{B} PRO B 26.204 18.383 MOTA 2219 N 97 34.900 26.011 17.493 1.00 22.89 В 2220 PRO B 97 33.744 MOTA CD PRO B 36.069 26.655 17.626 1.00 23.87 \mathbf{B} MOTA 2221 CA 97 1.00 22.81 \mathbf{B} MOTA 2222 CB PRO B 97 35.580 26.633 16.175 В 25.663 16.202 1.00 25.55 MOTA 2223 CG PRO B 97 34.411 В 36.498 28.061 18.021 1.00 23.80 MOTA 2224 C PRO B 97 В PRO B 97 35.665 28.905 18.353 1.00 24.40 MOTA 2225 0 В 28.307 17.990 1.00 22.02 MOTA 2226 N THR B 98 37.799 В 18.266 1.00 24.00 38.306 29.634 ATOM 2227 CA THR B 98 29.592 1.00 27.31 \mathbf{B} THR B 39.569 19.150 ATOM 2228 CB 98 1.00 35.69 В THR B 98 40.626 28.929 18.449 ATOM 2229 OG1 1.00 26.76 В 39.282 28.839 20.439 ATOM 2230 CG2 THR B 98 1.00 22.38 В 38.631 30.143 16.860 THR B 98 ATOM 2231 C 1.00 19.48 \mathbf{B} 39.376 29.504 16.116 THR B 98 ATOM 2232 0 31.274 1.00 21.55 В 38.041 16.487 2233 N VAL B 99 ATOM В 38.242 1.00 21.20 VAL B 31.824 15.152 99 ATOM 2234 CA 36.871 32.153 14.509 1.00 21.09 B VAL B MOTA 2235 CB 99 В 13.050 1.00 19.62 CG1 VAL B 99 37.043 32.541 ATOM 2236 В 30.944 14.625 1.00 18.29 CG2 VAL B 35.950 MOTA 2237 99 1.00 21.59 В VAL B 33.059 15.167 99 39.140 MOTA 2238 C 1.00 21.57 В VAL B 38.970 33.962 15.982 MOTA 2239 0 99 \mathbb{B} 1.00 22.65 THR B 100 33.084 14.252 MOTA 2240 N40.099 В 14.168 1.00 24.95 THR B 100 41.056 34.179 2241 CA MOTA В THR B 100 42.399 33.770 14.820 1.00 26.31 CB MOTA 2242 B33.321 1.00 30.10 2243 THR B 100 42.162 16.160 MOTA OG1 В 34.942 14.854 1.00 29.07 THR B 100 43.359 MOTA 2244 CG2 1.00 24.61 В 34.556 12.717 THR B 100 41.329 2245 C MOTA 1.00 23.89 В THR B 100 41.514 33.689 11.869 2246 ATOM 0 В 1.00 26.18 ILE B 101 41.363 35.852 12.435 ATOM 2247 N \mathbf{B} 1.00 29.32 41.638 36.315 11.080 ILE B 101 ATOM 2248 CA В 10.582 1.00 29.37 40.572 37.327 ILE B 101 ATOM 2249 CB В 9.231 1.00 29.49 CG2 ILE B 101 40.986 37.885 2250 ATOM \mathbb{B} 10.492 1.00 30.11 36.664 2251 CG1 ILE B 101 39.198 ATOM 1.00 29.81 В 37.605 10.002 CD1 ILE B 101 38.110 2252 ATOM В 42.988 37.015 11.040 1.00 31.04 ILE B 101 2253 C ATOM 1.00 31.24 В 37.868 11.877 2254 0 ILE B 101 43.270 MOTA В 1.00 34.47 **SER B 102** 36.664 10.066 43.820 ATOM 2255 N 37.303 9.940 1.00 39.17 В **SER B 102** 45.124 2256 CA ATOM В 36.617 1.00 37.33 **SER B 102** 46.143 10.844 **ATOM** 2257 CB 35.265 В 1.00 41.93 **SER B 102** 46.326 10.462 ATOM 2258 OG В 45.632 37.289 8.501 1.00 42.45 C 2259 SER B 102 MOTA 45.641 36.248 7.845 1.00 42.45 \mathbf{B} 0 SER B 102 ATOM 2260 В 7.988 1.00 45.38 N PRO B 103 46.052 38.455 ATOM 2261 \mathbf{B} 45.938 39.793 8.596 1.00 45.47 MOTA 2262 CD PRO B 103 \mathbf{B} 38.545 6.617 1.00 48.91 46.564 PRO B 103 ATOM 2263 CA В 6.312 46.446 40.032 1.00 47.74 ATOM 2264 CB PRO B 103 В 1.00 47.08 7.642 46.739 40.652 MOTA 2265 CG PRO B 103 \mathbf{B} 1.00 51.96 38.042 6.545 PRO B 103 48.010 2266 C ATOM \mathbf{B} 48.688 37.957 7.568 1.00 52.51 PRO B 103 ATOM 2267 0 B 1.00 55.84 48.475 37.699 5.346 2268 \mathbf{N} **SER B 104** ATOM \mathbf{B} 49.843 37.209 5.177 1.00 60.00 2269 CA SER B 104 ATOM B 50.018 36.578 3.791 1.00 59.60 ATOM 2270 CB SER B 104 В 37.520 2.759 1.00 59.05 ATOM 2271 SER B 104 49.778 OG В 5.368 1.00 63.75 50.842 38.353 ATOM 2272 C SER B 104 В 50.853 39.325 4.605 1.00 64.64 ATOM 2273 SER B 104 0 В 38.228 6.398 1.00 66.99 **ARG B 105** 51.677 ATOM 2274 N \mathbf{B} 52.674 6.736 1.00 69.17 39.242 MOTA 2275 CA ARG B 105 \mathbf{B} 53.631 38.700 7.808 1.00 70.33 2276 ARG B 105 MOTA CB В 54.672 37.690 7.318 1.00 72.24 2277 ARG B 105 ATOM CG В 6.449 1.00 73.51 54.073 36.586 ATOM 2278 CD ARG B 105 В 52.981 35.859 7.095 1.00 75.02 ATOM 2279 NE ARG B 105 \mathbf{B} 53.120 35.051 8.142 1.00 76.07 ATOM 2280 ARG B 105 ÇZ В 1.00 77.38 54.314 34.852 8.684 2281 ARG B 105 ATOM NHl \mathbf{B} 8.644 52.059 34.431 1.00 76.05 ATOM 2282 ARG B 105 NH2 \mathbf{B} 1.00 70.38 5.523 53.464 39.720 ATOM 2283 C ARG B 105 В 53.134 40.746 4.923 1.00 71.56 ARG B 105 ATOM 2284 0 46.629 \mathbf{B} 1.00 49.25 -1.86740.478 ATOM 2285 **ASN B 113** N В 46.963 40.039 -0.5151.00 48.42 ATOM 2286 CA**ASN B 113** В 0.477 1.00 51.23 46.726 41.181 MOTA 2287 CB **ASN B 113** В 1.00 53.89 47.268 40.875 1.863 ATOM **ASN B 113** 2288 CG \mathbf{B} 48.429 2.019 1.00 55.14 40.498 ATOM 2289 OD1 ASN B 113

ATOM	2290	ND2	ASN B	113	46.428	41.048	2.880	1.00 55.30	В
MOTA	2291	С	ASN B :	113	46.143	38.808	-0.118	1.00 45.78	В
ATOM	2292		ASN B	113	45.155	38.471	-0.774	1.00 44.99	В
ATOM	2293		LEU B		46.550	38.146	0.961	1.00 42.27	В
ATOM	2294			114	45.862	36.944	1.415	1.00 38.77	В
ATOM	2295			114	46.770	35.739	1.182	1.00 39.10	В
ATOM	2296			114	46.238	34.330	1.421	1.00 40.81	В
ATOM	2296			114	45.097	34.023	0.459	1.00 41.59	В
		=	•	114	47.379	33.341	1.222	1.00 41.03	В
ATOM	2298					36.986	2.883	1.00 36.39	В
ATOM	2299	C		114	45.424			1.00 35.98	В
ATOM	2300	0		114	46.237	37.204	3.783		
ATOM	2301			115	44.130	36.777	3.112	1.00 31.79	В
MOTA	2302	CA		115	43.576	36.766	4.460	1.00 28.77	В
ATOM	2303	CB		115	42.231	37.496	4.493	1.00 29.52	В
ATOM	2304	CG		115	42.156	38.843	5.218	1.00 30.12	В
MOTA	2305	CD1	LEU B	115	43.281	39.751	4.764	1.00 30.28	В
ATOM	2306	CD2	LEU B	115	40.799	39.479	4.951	1.00 28.39	В
MOTA	2307	C	LEU B	115	43.374	35.323	4.896	1.00 27.23	В
MOTA	2308	0	LEU B	115	42.815	34.513	4.154	1.00 25.72	В
MOTA	2309	N	VAL B	116	43.825	35.002	6.103	1.00 24.13	В
ATOM	2310	CA	VAL B	116	43.695	33.651	6.618	1.00 20.76	В
ATOM	2311	CB	VAL B	116	45.078	33.098	7.078	1.00 20.02	В
ATOM	2312	CG1	VAL B	116	44.915	31.757	7.777	1.00 17.46	В
ATOM	2313		VAL B		45.996	32.944	5.880	1.00 19.44	В
ATOM	2314	C	VAL B		42.723	33.568	7.784	1.00 20.38	В
ATOM	2315	0		116	42.860	34.293	8.766	1.00 19.54	В
ATOM	2316	И		117	41.724	32.701	7.669	1.00 20.87	В
ATOM	2317	CA		117	40.793	32.523	8.774	1.00 22.57	В
		CA		117	41.132	31.196	9.444	1.00 21.84	В
MOTA	2318	-				30.123	8.892	1.00 22.98	В
ATOM	2319	0	·	117 117	40.867		8.315	1.00 23.53	В
ATOM	2320	CB		117	39.332	32.486			
ATOM	2321	SG		117	38.217	32.222	9.734		В
ATOM	2322	N	SER B		41.728	31.277	10.627	1.00 19.87	В
MOTA	2323	CA		118	42.094	30.092	11.381	1.00 18.65	В
MOTA	2324	CB	SER B	118	43.345	30.356	12.226	1.00 19.67	B
ATOM	2325	OG	SER B	118	44.463	30.672	11.421	1.00 22.97	B
MOTA	2326	C	SER B	118	40.962	29.656	12.300	1.00 18.03	B
MOTA	2327	0	SER B	118	40.579	30.389	13.209	1.00 19.82	В
ATOM	2328	N	VAL B	119	40.426	28.463	12.050	1.00 17.57	В
ATOM	2329	CA	VAL B	119	39.365	27.889	12.874	1.00 15.30	В
ATOM	2330	CB	VAL B	119	38.202	27.364	12.006	1.00 15.69	В
ATOM	2331	CG1	VAL B	119	37.091	26.852	12.892	1.00 11.64	В
ATOM	2332	CG2	VAL B	119	37.695	28.484	11.076	1.00 13.82	В
ATOM	2333	C	VAL B	119	40.073	26.739	13.579	1.00 15.38	В
ATOM	2334	0	VAL B	119	40.318	25.680	12.992	1.00 16.76	B
ATOM	2335	N		120	40.404	26.958	14.844	1.00 16.03	В
ATOM	2336	CA		120	41.165	25.988	15.615	1.00 15.04	В
ATOM	2337	CB		120	42.487	26.613	16.031	1.00 13.75	В
MOTA	2338	OG1		120	42.221	27.713	16.915	1.00 17.84	В
ATOM	2339	CG2			43.230	27.144	14.815	1.00 12.18	В
			THR B		40.533	25.405	16.872	1.00 17.87	В
ATOM	2340	C			39.571	25.944	17.425	1.00 17.71	В
ATOM	2341	0	THR B			24.303		1.00 17.71	В
ATOM	2342	N		121	41.132		17.317		В
ATOM	2343	CA		121	40.738	23.576	18.511	1.00 20.97	
MOTA	2344	CB	ASP B		41.268	24.291	19.766	1.00 24.82	В
MOTA	2345	CG		121	42.797	24.330	19.831	1.00 31.04	В
ATOM	2346	OD1	ASP B	121	43.460	23.360	19.397	1.00 30.81	B
ATOM	2347	OD2	ASP B	121	43.339	25.333	20.346	1.00 34.38	B
MOTA	2348	C	ASP B	121	39.238	23.293	18.679	1.00 21.27	В
MOTA	2349	0	ASP B	121	38.629	23.671	19.683	1.00 23.00	В
ATOM	2350	N	PHE B	122	38.641	22.613	17.710	1.00 20.38	B
ATOM	2351	CA	PHE B	122	37.233	22.280	17.818	1.00 18.51	В
ATOM	2352	CB	PHE B	122	36.414	22.988	16.732	1.00 16.18	В
ATOM	2353	CG		122	36.817	22.644	15.319	1.00 13.31	В
ATOM	2354	CD1		122	37.695	23.463	14.615	1.00 11.43	В
ATOM	2355	CD2		122	36.247	21.547	14.664	1.00 10.93	В
ATOM	2356	CE1	PHE B	122	37.998	23.210	13.272	1.00 10.91	В
				122	36.541	21.280	13.317	1.00 12.31	B
MOTA	2357	CE2			37.419	22.118	12.618	1.00 12.31	В
ATOM	2358	CZ	PHE B		37.011	20.778	17.739	1.00 19.55	В
MOTA	2359	C		122				1.00 19.55	В
ATOM	2360	0	PHE B	122	37.889	20.029	17.301		В
ATOM	2361	N	TYR B		35.829	20.357	18.182	1.00 20.50	В
ATOM	2362	CA	TYR B		35.412	18.959	18.180	1.00 21.08	
ATOM	2363	CB	TYR B	123	36.067	18.201	19.340	1.00 19.11	В

ATOM	2364	CG	TYR B	123	35.919	16.702	19.228	1.00 18.56	В
ATOM	2365	CD1	TYR B	123	34.746	16.062	19.629	1.00 19.13	В
ATOM	2366	CE1	TYR B	123	34.572	14.695	19.446	1.00 17.75	В
MOTA	2367	CD2	TYR B	123	36.920	15.932	18.647	1.00 17.20	В
ATOM	2368	CE2	TYR B	123	36.762	14.566	18.455	1.00 17.38	B
ATOM	2369	CZ	TYR B	123	35.584	13.953	18.853	1.00 19.59	В
MOTA	2370	OH	TYR B	123	35.412	12.608	18.631	1.00 22.32	В
MOTA	2371	C	TYR B	123	33.896	18.957	18.351	1.00 21.83	В
MOTA	2372	0	TYR B	123	33.365	19.708	19.165	1.00 23.26	B
ATOM	2373	N		124	33.175	18.126	17.584	1.00 21.65	В
ATOM	2374	CD		124	31.725	17.996	17.808	1.00 23.81	B
ATOM	2375	CA		124	33.627	17.177	16.562	1.00 22.30	В
ATOM	2376	CB	PRO B	124	32.398	16.290	16.353	1.00 21.95	В
ATOM	2377	CG	PRO B	124	31.270	17.237	16.586	1.00 23.07	В
ATOM	2378	C	PRO B	124	34.128	17.813	15.266	1.00 22.20 1.00 24.43	B B
ATOM	2379	0	PRO B	124	34.204	19.035 16.971	15.149 14.291	1.00 24.43	В
ATOM	2380	N CA		125 125	34.457 34.987	17.428	13,007	1.00 20.03	В
ATOM	2381 2382	CB	ALA B		35.571	16.236	12.244	1.00 20.20	В
MOTA MOTA	2382	CD		125	34.057	18.222	12.078	1.00 22.42	В
ATOM	2384	0		125	34.512	19.129	11.400	1.00 24.48	В
ATOM	2385	N	GLN B	126	32,772	17.893	12.036	1.00 25.59	B
ATOM	2386	CA	GLN B		31.845	18.598	11.147	1.00 27.46	В
ATOM	2387	CB	GLN B		30.414	18,101	11.357	1.00 29.99	В
ATOM	2388	CG	GLN B	126	30.283	16.595	11.480	1.00 36.21	В
ATOM	2389	CD	GLN B		30.625	16.102	12.870	1.00 38.28	В
ATOM	2390	OE1	GLN B	126	30.558	14.905	13.158	1.00 40.46	В
ATOM	2391	NE2	GLN B	126	30.989	17.030	13.745	1.0040.92	В
ATOM	2392	C	GLN B	126	31.876	20.112	11.333	1.00 28.28	В
ATOM	2393	0		126	31.571	20.627	12.410	1.00 29.36	В
ATOM	2394	N	ILE B	127	32.221	20.831	10.273	1.00 27.17	В
MOTA	2395	CA	ILE B	127	32.292	22.279	10.353	1.00 27.02	В
ATOM	2396	CB	ILE B	127	33.656	22.716	10.931	1.00 27.21	В
ATOM	2397	CG2	ILE B	127	34.767	22.453	9.898	1.00 21.63	В
ATOM	2398	CG1	ILE B	127	33.612	24.195	11.316	1.00 24.63	В
ATOM	2399	CD1	ILE B	127	34.760	24.633	12.198	1.00 25.86	В
ATOM	2400	C	ILE B	127	32.117	22.903	8.969	1.00 27.10	В
ATOM	2401	0	ILE B	127	32.393	22.258	7.956	1.00 26.58	В
ATOM	2402	N	LYS B	128	31.666	24.155	8.940	1.00 25.41	В
MOTA	2403	CA	LYS B	128	31.457	24.884	7.689	1.00 27.45	В
ATOM	2404	CB	LYS B	128	29.964	24.927	7.334	1.00 29.68	В
MOTA	2405	CG	LYS B	128	29.633	25.685	6.046	1.00 34.69	В
ATOM	2406	CD	LYS B		30.129	24.954	4.793	1.00 38.25	В
ATOM	2407	CE	LYS B		29.802	25.742	3.517	1.00 40.20	B B
ATOM	2408	NZ	LYS B		30.281	25.071	2.271 7.861	1.00 39.87 1.00 25.41	В
ATOM	2409	C	LYS B		31.983	26.301 27.019	8.759	1.00 25.41	В
ATOM	2410	O NT	LYS B VAL B		31.559 32.911	26.700	7.002	1.00 25.70	В
MOTA	2411	N CA	VAL B		33.493	28.034	7.078	1.00 24.82	В
MOTA MOTA	2412 2413	CB	VAL B		35.013	27.956	7.329	1.00 24.17	В
ATOM	2413		VAL B		35.592	29.351	7.452	1.00 22.14	В
ATOM	2414	CG2			35.295	27.136	8.583	1.00 22.44	В
ATOM	2416	C	VAL B		33.248	28.791	5.778	1.00 25.17	В
ATOM	2417	0	VAL B		33.532	28.283	4.701	1.00 25.50	В
MOTA	2418	N	ARG B		32.724	30.007	5.884	1.00 27.21	В
ATOM	2419	CA	ARG B		32.445	30.814	4.701	1.00 28.49	В
ATOM	2420	CB		130	30.931	30.920	4.470	1.00 31.77	В
ATOM	2421	CG	ARG B	130	30.239	29.591	4.183	1.00 34.92	В
ATOM	2422	CD	ARG B	130	28.927	29.813	3.432	1.00 41.30	В
ATOM	2423	NE	ARG B	130	27.834	30.254	4.291	1.00 42.15	В
MOTA	2424	CZ	ARG B	130	27.032	29.426	4.953	1.00 46.05	В
MOTA	2425	NH1	ARG B	130	27.200	28.112	4.849	1.00 45.50	В
ATOM	2426	NH2	ARG B	130	26.061	29.910	5.718	1.00 48.30	В
MOTA	2427	C	ARG B	130	33.036	32.211	4.792	1.00 27.57	В
ATOM	2428	0	ARG B	130	33.130	32.789	5.874	1.00 26.00	В
MOTA	2429	N	TRP B	131	33.440	32.744	3.645	1.00 27.37	В
MOTA	2430	CA	TRP B		34.004	34.085	3.571	1.00 30.27	В
MOTA	2431	CB	TRP B		35.281	34.083	2.737	1.00 30.21	В
MOTA	2432	CG	TRP B		36.532	33.844	3.521	1.00 32.32	В
MOTA	2433	CD2			37.155	34.757	4.432	1.00 32.41	B B
ATOM	2434	CE2			38.334	34.142	4.900	1.00 33.07	В
ATOM	2435	CE3			36.831	36.039	4.897	1.00 31.75 1.00 32.80	В
ATOM	2436	CD1			37.333	32.741	3.478	1.00 32.80	B
MOTA	2437	NE1	TRP B	131	38.420	32.913	4.300	T.00 3T.33	<i>ن</i>

ATOM	2438	CZ2	TRP B	131	39.193	34.764	5.812	1.00 32.82	В
ATOM	2439	CZ3		131	37.680	36.656	5.800	1.00 32.08	В
ATOM	2440	CH2		131	38.849	36.017	6.249	1.00 33.40	В
				131	33.003	35.064	2.949	1.00 32.99	В
ATOM	2441	C							В
MOTA	2442	0		131	32.367	34.759	1.940	1.00 32.18	
MOTA	2443	N		132	32.879	36.242	3.550	1.00 35.48	В
ATOM	2444	CA	PHE B	132	31.962	37.263	3.058	1.00 39.35	В
MOTA	2445	CB	PHE B	132	30.856	37.501	4.077	1.00 38.14	В
ATOM	2446	CG	PHE B	132	29.843	36.407	4.123	1.00 38.39	В
ATOM	2447	CD1	PHE B	132	28.804	36.373	3.202	1.00 38.31	В
ATOM	2448	CD2		132	29.930	35.399	5.075	1.00 38.21	В
ATOM	2449	CE1		132	27.860	35.348	3.229	1.00 39.26	В
					28.992	34.369	5.111	1.00 38.83	В
ATOM	2450	CE2		132					
MOTA	2451	CZ		132	27.954	34.345	4.184		В
MOTA	2452	C		132	32.650	38.583	2.755	1.00 41.59	В
ATOM	2453	0	PHE B	132	33.515	39.025	3.508	1.00 42.72	B
ATOM	2454	N	ARG B	133	32.267	39.203	1.640	1.00 45.04	B
ATOM	2455	CA	ARG B	133	32.829	40.490	1.242	1.00 48.28	В
ATOM	2456	CB	ARG B	133	32.510	40.787	-0.227	1.00 51.68	В
ATOM	2457	CG		133	33.293	41.958	-0.829	1.00 55.78	В
ATOM	2458	CD		133	34.787	41.655	-0.867	1.00 57.07	В
				133	35.580	42.741	-1.440	1.00 59.30	В
ATOM	2459	NE						1.00 60.93	В
ATOM	2460	CZ		133	35.523	43.135	-2.710		
ATOM	2461	NHI		133	34.702	42.536	-3.564	1.00 61.44	В
MOTA	2462	NH2	ARG B	133	36.295	44.132	-3.128	1.00 61.77	В
MOTA	2463	C	ARG B	133	32.129	41.492	2.145	1.00 49.07	В
ATOM	2464	0	ARG B	133	32.299	41.460	3.358	1.00 51.26	В
ATOM	2465	N	ASN B	134	31.331	42.376	1.572	1.00 49.23	В
ATOM	2466	CA	ASN B		30.614	43.336	2.393	1.00 48.83	В
ATOM	2467	CB	ASN B		30.582	44.702	1.710	1.00 45.93	В
					31.973	45.290	1.523	1.00 45.10	В
ATOM	2468	CG	ASN B					1.00 41.81	В
MOTA	2469	OD1			32.450	45.440	0.397		
ATOM	2470	ND2	ASN B		32.634	45.618	2.634	1.00 41.82	В
MOTA	2471	C	asn b	134	29.203	42.795	2.594	1.00 50.25	В
ATOM	2472	0	ASN B	134	28.222	43.529	2.508	1.00 52.28	B
ATOM	2473	N	ASP B	135	29.122	41.496	2.868	1.00 50.15	В
ATOM	2474	CA	ASP B	135	27.847	40.819	3.072	1.00 51.07	В
ATOM	2475	C	ASP B	135	27.590	39.855	1.910	1.00 51.76	В
ATOM	2476	0	ASP B		26.586	39.136	1.893	1.00 51.82	В
			GLN B		28.507	39.856	0.944	1.00 50.97	В
ATOM	2477	N				38.999	-0.240	1.00 51.24	В
MOTA	2478	CA		136	28.421				
MOTA	2479	CB	7	136	28.766	39.805	-1.493	1.00 53.78	B
ATOM	2480	CG	GLN B	136	28.736	39.000	-2.783	1.00 58.16	В
ATOM	2481	CD	GLN B	136	29.675	39.559	-3.839	1.00 59.39	В
ATOM	2482	OE1	GLN B	136	30.895	39.527	-3.675	1.00 60.12	В
MOTA	2483	NE2	GLN B	136	29.110	40.078	-4.926	1.00 59.45	В
ATOM	2484	С	GLN B	136	29.395	37.825	-0.124	1.00 49.46	В
ATOM	2485	Ō	GLN B		30.607	38.026	-0.035	1.00 48.29	В
ATOM	2486	N		137	28.873	36.603	-0.144	1.00 47.64	В
			GLU B		29.730	35.432	-0.027	1.00 46.85	В
ATOM	2487	CA						1.00 47.17	В
MOTA	2488	СВ	GLU B		28.899	34.152	0.022		
MOTA	2489	CG	GLU B		29.695	32.975	0.556	1.00 50.22	В
ATOM	2490	CD	GLU B		28.866	31.726	0.743	1.00 52.65	В
MOTA	2491	OE1	GLU B	137	27.699	31.842	1.171	1.00 55.57	В
MOTA	2492	OE2	GLU B	137	29.391	30.623	0.478	1.00 54.41	В
ATOM	2493	С	GLU B	137	30.755	35.320	-1.149	1.00 45.23	В
ATOM	2494	0	GLU B		30.445	35.544	-2.314	1.00 45.04	В
ATOM	2495	N	GLU B		31.983	34.977	-0.776	1.00 44.63	В
				138	33.078	34.808	-1.724	1.00 44.36	В
ATOM	2496	CA						1.00 45.65	В
MOTA	2497	CB	GLU B		34.284	35.658	-1.307		
MOTA	2498	CG	GLU B		34.076	37.166	-1.320	1.00 48.42	В
MOTA	2499	CD	GLU B	138	34.144	37.761	-2.717	1.00 50.71	В
MOTA	2500	OE1	GLU B	138	35.120	37.471	-3.442	1.00 51.60	В
ATOM	2501	OE2	GLU B	138	33.227	38.526	-3.086	1.00 50.99	В
ATOM	2502	C		1.38	33.498	33.335	-1.740	1.00 43.68	В
ATOM	2502	0	GLU B		33.831	32.769	-0.697	1.00 43.53	В
ATOM	2503	N	THR B	139	33.468	32.711	-2.914	1.00 42.58	В
			THR B	139	33.400	31.313	-3.044	1.00 41.76	В
ATOM	2505	CA			32.739	30.415	-3.543	1.00 41.04	В
ATOM	2506	CB	THR B	139					В
ATOM	2507	OG1			32.207	30.948	-4.759	1.00 40.71	
ATOM	2508	CG2		139	31.641	30.325	-2.492	1.00 41.89	В
ATOM	2509	C	THR B		35.038	31.245	-4.026	1.00 40.93	В
ATOM	2510	0	THR B	139	35.855	30.326	-3.981	1.00 40.04	В
ATOM	2511	N	ALA B	140	35.096	32.224	-4.920	1.00 40.67	В
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ATOM	2512	CA	ALA B 1	40	36.179	32.305	-5.887	1.00 41.22	В
ATOM	2513	CB	ALA B 1	.40	35.714	33.016	-7.158	1.00 41.13	B
ATOM	2514	C	ALA B 1	40	37.247	33.126	-5.177	1.00 41.09	В
ATOM	2515	0	ALA B 1	.40	36.976	34.232	-4.693	1.00 43.11	В
ATOM	2516	N	GLY B 1	.41	38.455	32.582	-5.102	1.00 39.60	В
ATOM	2517	CA	GLY B 1		39.526	33.278	-4.418	1.00 35.11	В
ATOM	2518	C	GLY B 1		39.739	32,651	-3.051	1.00 33.42	В
ATOM	2519	0		41	40.605	33.076	-2.287	1.00 31.24	В
ATOM	2520	И		L42	38.945	31.628	-2.750	1.00 31.89	В
ATOM	2521	CA		L42	39.033	30.937	-1.470	1.00 32.27	В
ATOM	2521	CB		L 1 2	37.645	30.790	-0.813	1.00 31.90	В
		CG1		L42 L42	37.733		0.400	1.00 32.37	В
MOTA	2523	CG2		L42 L42	37.735	32.161	-0.402	1.00 32.57	В
ATOM	2524							1.00 32.33	В
ATOM	2525	C		L42	39.652	29.552	-1.564		
ATOM	2526	0		L42	39.211	28.712	-2.343	1.00 32.44	В
ATOM	2527	N		L43	40.676	29.326	-0.752	1.00 30.76	В
ATOM	2528	CA		L43	41.357	28.045	-0.702	1.00 29.79	В
ATOM	2529	CB		L43	42.815	28.154	-1.162	1.00 29.63	В
ATOM	2530	CG1		L 4 3	43.439	26.768	-1.212	1.00 31.60	B
ATOM	2531	CG2		L43	42.885	28.819	-2.514	1.00 33.43	B
ATOM	2532	С	VAL B 1	L43	41.357	27.575	0.749	1.00 30.61	В
MOTA	2533	0	VAL B 1	L43	41.665	28.338	1.667	1.00 28.64	В
MOTA	2534	N	SER B 1	L44	41.017	26.313	0.950	1.00 29.65	B
ATOM	2535	CA	SER B 3	L44	40.970	25.756	2.282	1.00 28.42	В
ATOM	2536	CB	SER B	L 44	39.541	25.325	2.605	1.00 29.23	В
MOTA	2537	OG	SER B	L 44	39.457	24.705	3.875	1.00 33.81	В
ATOM	2538	C	SER B 1	L44	41.900	24.562	2.373	1.00 27.32	В
MOTA	2539	0	SER B 1	L44	42.101	23.840	1.397	1.00 27.40	В
ATOM	2540	N	THR B	L 4 5	42.492	24.372	3.542	1.00 25.70	В
ATOM	2541	CA	THR B 1	L45	43.364	23.227	3.755	1.00 24.82	В
ATOM	2542	CB	THR B	145	44.272	23.418	4.995	1.00 25.01	В
ATOM	2543	OG1	THR B	145	43.467	23.399	6.186	1.00 25.18	В
ATOM	2544	CG2		145	45.022	24.743	4.923	1.00 23.27	В
ATOM	2545	C		145	42.392	22.100	4.071	1.00 24.16	В
ATOM	2546	0		145	41.200	22.335	4.272	1.00 23.86	В
ATOM	2547	N		146	42.865	20.854	4.081	1.00 23.17	В
ATOM	2548	CD		146	44.116	20.231	3.618	1.00 22.29	В
ATOM	2549	CA		146	41.854	19.852	4.419	1.00 23.18	В
ATOM	2550	CB		146	42.521	18.536	4.008	1.00 24.20	В
ATOM	2551	CG		146	43.998	18.833	4.162	1.00 22.82	В
		C		146	41.597	19.945	5.933	1.00 22.63	В
ATOM	2552			146	42.213	20.766	6.625	1.00 21.32	В
ATOM	2553	O 74			40.667	19.146	6.445	1.00 22.60	В
ATOM	2554	N	LEU B			19.140	7.883	1.00 22.34	В
ATOM	2555	CA		147	40.414	18.216	8.213	1.00 22.34	В
ATOM	2556	CB		147	39.241		9.691	1.00 22.17	В
ATOM	2557	CG		147	38.934	17.973			В
ATOM	2558	CD1		147	38.629	19.288	10.368		
MOTA	2559	CD2			37.746	17.026	9.826	1.00 25.55	В
ATOM	2560	C	LEU B		41.710	18.609	8.515	1.00 21.99	В
ATOM	2561	0	LEU B :		42.290	17.640	8.024	1.00 21.35	В
ATOM	2562	N	ILE B		42.175		9.581	1.00 20.48	В
ATOM	2563	CA	ILE B		43.406	18.813	10.228	1.00 19.15	B
ATOM	2564	CB	ILE B		44.392	19.990	10.403	1.00 21.68	В
ATOM	2565	CG2			45.666	19.505	11.065	1.00 20.10	В
ATOM	2566	CG1			44.728	20.609		1.00 25.04	В
ATOM	2567	CD1			45.416	19.649		1.00 29.06	В
MOTA	2568	C	ILE B	148	43.160	18.208	11.603	1.00 17.56	В
MOTA	2569	0	ILE B	148	42.566	18.852	12.467	1.00 14.88	В
MOTA	2570	N	ARG B	149	43.625	16.973	11.795	1.00 15.95	В
MOTA	2571	CA	ARG B	149	43.492	16.273	13.077	1.00 17.47	. B
MOTA	2572	CB	ARG B	149	43.420	14.763	12.852	1.00 16.94	В
MOTA	2573	CG	ARG B	149	43.202	13.941	14.128	1.00 20.29	В
ATOM	2574	CD	ARG B	149	43.252	12.448	13.821		В
ATOM	2575	NE	ARG B		42.168	12.028	12.938	1.00 21.97	В
ATOM	2576	CZ	ARG B		40.934	11.742	13.348	1.00 23.22	В
ATOM	2577	NH1			40.015	11.374	12.471	1.00 23.89	В
ATOM	2578	NH2			40.623	11.803	14.636		В
ATOM	2579	C	ARG B		44.720	16.603	13.937	1.00 17.66	В
ATOM	2579	0	ARG B		45.850	16.311	13.549		В
ATOM	2580	N	ASN B		44.496	17.210	15.098	1.00 16.67	В
	2581	CA	ASN B		45.592	17.593	15.980	1.00 16.94	В
ATOM		CA	ASN B		45.174	18.756	16.890	1.00 15.38	В
MOTA	2583		ASN B		44.899	20.034	16.118	1.00 18.41	В
MOTA	2584	CG		150					В
ATOM	2585	OD1	. מייאט	·	005	20.300	. .		

ATOM	2586	ND2	ASN I	3 150	43.790	20.691	16.440	1.00 17.88	В
		C		3 150	46.116	16.452	16.841	1.00 18.47	B
ATOM	2587								
ATOM	2588	0	ASN I	3 150	47.220	16.540	17.384	1.00 17.03	В
ATOM	2589	N	GLY I	3 151	45.324	15.391	16.968	1.00 17.77	В
ATOM	2590	CA	GLY I	3 151	45.734	14.251	17.770	1.00 19.16	В
MOTA	2591	C	GLY I		45.258	14.293	19.213	1.00 20.44	В
ATOM	2592	0	GLY I	3 151	45.198	13.264	19.877	1.00 22.31	В
ATOM	2593	N	ASP I	3 152	44.906	15.475	19.701	1.00 20.79	В
MOTA	2594	CA		3 152	44.450	15.624	21.077	1.00 21.97	В
ATOM	2595	CB	ASP I	3 152	45.192	16.790	21.748	1.00 21.95	В
MOTA	2596	CG	ASP I	3 152	45.027	18.101	20.992	1.00 28.05	В
				3 152	45.764	19.060	21.300	1.00 30.94	В
ATOM	2597	OD1							
ATOM	2598	QD2	ASP I	3 152	44.158	18.181	20.090	1.00 28.02	В
ATOM	2599	C	ASP I	3 152	42.939	15.847	21.175	1.00 20.51	В
ATOM	2600	0		3 152	42.474	16.619	22.010	1.00 21.63	В
ATOM	2601	N		3 153	42.183	15.166	20.322	1.00 19.19	В
MOTA	2602	CA	TRP I	3 153	40.724	15.278	20.300	1.00 16.82	В
ATOM	2603	CB	TRP I	3 153	40.121	14.865	21.657	1.00 15.80	В
							22.005	1.00 16.21	В
ATOM	2604	CG		3 153	40.326	13.408			
ATOM	2605	CD2	TRP I	3 153	39.415	12.322	21.756	1.00 16.58	В
ATOM	2606	CE2	TRP I	3 153	40.047	11.134	22.188	1.00 15.08	В
ATOM	2607	CE3	TRP I	3 153	38.125	12.238	21.211	1.00 15.69	В
ATOM	2608	CDI	TRP I	3 153	41.435	12.848	22.564	1.00 14.68	B
MOTA	2609	NE1	TRP I	3 153	41.278	11.483	22.677	1.00 15.53	В
ATOM	2610	CZ2	TRP F	3 153	39.438	9.879	22.087	1.00 15.60	В
									В
MOTA	2611	CZ3		3 153	37.518	10.987	21.112	1.00 14.22	
MOTA	2612	CH2	TRP 1	B 1 53	38.176	9.827	21.549	1.00 13.89	В
ATOM	2613	C	TRP I	B 153	40.194	16.660	19.890	1.00 16.09	В
				3 153	39.159	17.110	20.379	1.00 14.28	В
ATOM	2614	0							
ATOM	2615	N	THR I	3 154	40.929	17.342	19.020	1.00 15.11	В
ATOM	2616	CA	THR I	B 154	40.499	18.627	18.483	1.00 16.19	В
ATOM	2617	CB	ו קאיזי	3 154	41.176	19.877	19.150	1.00 18.02	В
ATOM	2618	OG1	THR I	B 154	42.602	19.804	19.008	1.00 19.50	В
MOTA	2619	CG2	THR I	B 154	40.788	20.000	20.608	1.00 15.03	В
ATOM	2620	С	THR 1	B 154	40.908	18.602	17.024	1.00 15.24	В
						17.832	16.635	1.00 15.24	В
ATOM	2621	0		B 154	41.773				
MOTA	2622	N	PHE]	B 155	40.269	19.437	16.220	1.00 18.04	В
ATOM	2623	CA	PHE I	B 155	40.577	19.538	14.801	1.00 16.03	В
ATOM	2624	CB		B 155	39.404	19.042	13.938	1.00 16.98	В
MOTA	2625	CG	PHE]	B 155	39.069	17.579	14.118	1.00 17.58	В
ATOM	2626	CD1	PHE 1	B 155	38.133	17.170	15.074	1.00 18.20	В
ATOM	2627	CD2	PHE	B 155	39.670	16.611	13.312	1.00 17.71	В
									В
MOTA	2628	CE1		B 155	37.799	15.810	15.223	1.00 17.81	
MOTA	2629	CE2	PHE :	B 155	39.346	15.250	13.451	1.00 17.57	B
MOTA	2630	CZ	PHE :	B 155	38.407	14.849	14.409	1.00 16.39	В
		C		B 155	40.793	21.015	14.503	1.00 16.67	В
ATOM	2631								
MOTA	2632	0	PHE :	B 155	40.532	21.870	15.352	1.00 16.84	В
ATOM	2633	N	GLN :	B 156	41.281	21.312	13.304	1.00 14.72	В
ATOM	2634	CA	GLN :	B 156	41.467	22.689	12.886	1.00 14.66	В
								1.00 16.69	В
ATOM	2635	CB		B 156	42.811	23.264	13.357		
MOTA	2636	CG	GLN :	B 156	44.039	22.698	12.669	1.00 15.65	В
ATOM	2637	$^{\rm CD}$	GLN :	B 156	45.292	23.486	13.011	1.00 17.87	В
ATOM	2638	OE1	GLN :	B 156	45.477	24.617	12.555	1.00 17.56	В
MOTA	2639	NE2	GLN :	B 156	46.153	22.897	13.830	1.00 15.40	В
ATOM	2640	C	GLN :	B 156	41.398	22.722	11.371	1.00 14.00	В
ATOM	2641	0	GLN :	B 156	41.477	21.691	10.716	1.00 15.17	В
			ILE :		41.241	23.911	10.818	1.00 15.34	В
MOTA	2642	N							
MOTA	2643	CA	ILE :	B 157	41.165	24.057	9.383	1.00 17.26	В
ATOM	2644	CB	ILE	B 157	39.791	23.585	8.856	1.00 16.56	В
ATOM	2645	CG2	TT.E	B 157	38.675	24.429	9.474	1.00 13.07	В
			·						
MOTA	2646	CG1			39.765	23.649	7.326	1.00 17.72	В
MOTA	2647	CD1	ILE :	B 157	38.583	22.913	6.712	1.00 14.50	В
ATOM	2648	C	ILE	B 157	41.379	25.523	9.074	1.00 18.67	В
				B 157	40.823	26.391	9.745	1.00 22.28	В
ATOM	2649	0							
ATOM	2650	N		B 158	42.217	25.795	8.083	1.00 18.98	В
MOTA	2651	CA	LEU	B 158	42.508	27.162	7.690	1.00 20.77	В
MOTA	2652	CB		в 158	44.022	27.368	7.555	1.00 22.23	В
								1.00 26.12	
ATOM	2653	CG		B 158	44.851	27.525	8.838		В
MOTA	2654	CD1	LEU	B 158	44.689	26.320	9.740	1.00 29.01	В
MOTA	2655	CD2	LEU	B 158	46.311	27.701	8.465	1.00 28.46	В
		C		B 158	41.817	27.484	6.371	1.00 20.61	В
ATOM	2656	-							
MOTA	2657	0		B 158	41.934	26.734	5.401	1.00 19.39	В
MOTA	2658	N	VAL	B 159	41.088	28.596	6.346	1.00 21.67	В
ATOM	2659	CA	VAL	B 159	40.380	29.011	5.141	1.00 21.90	В
			. —						_

ATOM	2660	CB	VAL	В	159	38.855	29.061	5.365	1.00 22.06	В
ATOM	2661	CG1	VAL	В	159	38.147	29.252	4.043	1.00 20.55	В
ATOM	2662	CG2	VAL	В	159	38.381	27.766	6.009	1.00 20.83	В
ATOM	2663	C		В	159	40.899	30.379	4.749	1.00 21.80	В
									1.00 20.82	В
ATOM	2664	0	VAL		159	40.721	31.357	5.473		
ATOM	2665	N		В	160	41.555	30.416	3.592	1.00 23.56	B
ATOM	2666	CA	MET	В	160	42.179	31.613	3.055	1.00 25.12	В
ATOM	2667	CB	MET	В	160	43.580	31.257	2.559	1.00 26.80	В
MOTA	2668	CG	MET	В	160	44.479	30.736	3.678	1.00 32.00	В
ATOM	2669	SD	MET	В	160	45.850	29.700	3.145	1.00 38.02	В
ATOM	2670	CE	MET	В	160	45.094	28.065	3.307	1.00 35.43	В
ATOM	2671	C		В	160	41.387	32.269	1.941	1.00 28.27	В
ATOM	2672	0		В	160	40.684	31.602	1.177	1.00 28.76	В
ATOM	2673	N		В	161	41.518	33.588	1.854	1.00 29.59	В
MOTA	2674	CA	LEU	В	161	40.820	34.366	0.845	1.00 32.69	В
MOTA	2675	CB	LEU	B	161	39.669	35.142	1.487	1.00 30.80	В
ATOM	2676	CG	LEU	В	161	39.031	36.199	0.586	1.00 31.56	В
ATOM	2677	CD1	LEU	В	161	38.156	35.516	-0.460	1.00 29.64	В
ATOM	2678	CD2	LEU	В	161	38.213	37.167	1.423	1.00 29.89	В
ATOM	2679	C		В	161	41.755	35.349	0.154	1.00 35.59	В
				В	161	42.350	36.216	0.801	1.00 35.54	В
ATOM	2680	0								
ATOM	2681	N		B	162	41.895	35.203	-1.158	1.00 39.87	В
MOTA	2682	CA	GLU		162	42.728	36.118	-1.927	1.00 44.05	В
ATOM	2683	CB	GLU	В	162	42.995	35.565	-3.331	1.00 46.86	В
ATOM	2684	CG	GLU	\mathbf{B}	162	43.795	36.497	-4.239	1.00 50.98	В
ATOM	2685	CD	GLU	В	162	45.274	36.537	-3.891	1.00 54.75	В
ATOM	2686	OE1	GLU	В	162	45.604	36.802	-2.715	1.00 56.53	В
ATOM	2687	OE2	GLU		162	46.108	36.308	-4.796	1.00 55.16	В
		C	GLU		162	41.879	37.372	-2.029	1.00 44.69	В
ATOM	2688									
ATOM	2689	0		В	162	40.719	37.302	-2.434	1.00 44.39	В
MOTA	2690	N	MET	В	163	42.436	38.514	-1.648	1.00 46.67	B
MOTA	2691	CA	MET	В	163	41.670	39.746	-1.716	1.00 49.56	В
MOTA	2692	CB	MET	В	163	40.881	39.949	-0.412	1.00 51.22	В
ATOM	2693	CG	MET	В	163	41.652	39.675	0.876	1.00 51.58	В
ATOM	2694	SD	MET	В	163	42.910	40.901	1.274	1.00 56.87	В
ATOM	2695	CE		В	163	41.915	42.187	2.029~	1.00 54.89	В
ATOM	2696	C		В	163	42.487	40.986	-2.028	1.00 51.43	В
		0		В	163	43.717	40.988	-1.942	1.00 51.02	B
ATOM	2697								1.00 51.02	В
ATOM	2698	N	THR		164	41.777	42.038	-2.412		
ATOM	2699	CA	THR		164	42.385	43.316	-2.738	1.00 56.61	B
ATOM	2700	CB	THR	В	164	41.889	43.820	-4.116	1.00 57.48	В
MOTA	2701	OG1	THR	В	164	40.457	43.744	-4.172	1.00 57.81	В
MOTA	2702			R	164	42.480	42.967	-5.234	1.00 57.23	В
ATOM	2102	CG2	THR							
		CG2 C	THR		164	42.012	44.318	-1.642	1.00 57.80	В
ATOM	2703	C	THR	В		42.012		-1.642	1.00 57.80	
ATOM ATOM	2703 2704	C 0	THR THR	B B	164	42.012 40.866	44.766	-1.642 -1.555	1.00 57.80 1.00 57.08	B B
ATOM	2703 2704 2705	0 N	THR THR PRO	B B B	164 165	42.012 40.866 42.976	44.766 44.658	-1.642 -1.555 -0.770	1.00 57.80 1.00 57.08 1.00 58.98	В В В
ATOM ATOM	2703 2704 2705 2706	C O N CD	THR THR PRO PRO	B B B	164 165 165	42.012 40.866 42.976 44.315	44.766 44.658 44.055	-1.642 -1.555 -0.770 -0.647	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54	В В В
ATOM ATOM ATOM	2703 2704 2705 2706 2707	C O N CD CA	THR THR PRO PRO PRO	B B B B	164 165 165 165	42.012 40.866 42.976 44.315 42.734	44.766 44.658 44.055 45.605	-1.642 -1.555 -0.770 -0.647 0.322	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52	B B B B
ATOM ATOM	2703 2704 2705 2706	C O N CD	THR THR PRO PRO PRO PRO	B B B B	164 165 165 165 165	42.012 40.866 42.976 44.315 42.734 44.063	44.766 44.658 44.055 45.605 45.608	-1.642 -1.555 -0.770 -0.647 0.322 1.078	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33	B B B B
ATOM ATOM ATOM	2703 2704 2705 2706 2707	C O N CD CA	THR THR PRO PRO PRO PRO	B B B B	164 165 165 165	42.012 40.866 42.976 44.315 42.734	44.766 44.658 44.055 45.605	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42	B B B B
ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708	C O N CD CA CB	THR THR PRO PRO PRO PRO	B B B B B B	164 165 165 165 165	42.012 40.866 42.976 44.315 42.734 44.063	44.766 44.658 44.055 45.605 45.608	-1.642 -1.555 -0.770 -0.647 0.322 1.078	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65	B B B B
ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709	C O N CD CA CB CG	THR THR PRO PRO PRO PRO PRO	B B B B B B B	164 165 165 165 165 165	42.012 40.866 42.976 44.315 42.734 44.063 44.604	44.766 44.658 44.055 45.605 45.608 44.236	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42	B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711	C O N CD CA CB CG	THR THR PRO PRO PRO PRO PRO PRO	B B B B B B B B	164 165 165 165 165 165	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347	44.766 44.658 44.055 45.605 45.608 44.236 47.002	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65	B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712	CONCACE	THR THR PRO PRO PRO PRO PRO PRO PRO PRO	B B B B B B B B B B	164 165 165 165 165 165 165 165	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45	B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713	CONCACGONCA	THR THR PRO PRO PRO PRO PRO PRO GLN GLN	B B B B B B B B B B B	164 165 165 165 165 165 165 165 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32	B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714	CONCACBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN	B B B B B B B B B B B B B B B B B B B	164 165 165 165 165 165 165 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46	B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715	CONCACBCCONCACCBCCCCCCCCCCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN	B B B B B B B B B B B B B B B B B B B	164 165 165 165 165 165 165 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00	B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716	CONCACBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19	B B B B B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715	CONCACBCCCONCACCBCCCONCACCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.945 47.942 47.448	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48	B B B B B B B B B B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716	CONCACBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717	CONCACBCCCONCACCBCCCONCACCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.945 47.942 47.448	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48	B B B B B B B B B B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719	CONCACBCCONCACBCCCONCACCBCCCCCCCCCCCCCCC	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.945 47.448 48.492	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720	CONCACE CONCACE CONE CONE CONE CONCACE CONE CONE CONE CONE CONE CONE CONE CO	THR THR PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN GLN GLN GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.893 39.021	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721	CONCACE CONCAC	THR THR PRO PRO PRO PRO PRO GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.021 40.266	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.945 47.448 48.492 49.287 48.635 50.501	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 62.65 1.00 62.16	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722	CONCACGONACONCA	THR THR PRO PRO PRO PRO PRO GLN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.617 39.893 39.021 40.266 39.645	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.945 47.448 48.492 49.287 48.635 50.501 51.111	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.16 1.00 60.86	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723	CONCACONCACONCACE	THR PRO PRO PRO PRO PRO PRO GLN GLN GLN GLN GLN GLN ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.893 39.021 40.266 39.645 40.190	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.57	B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724	CONCABG CONCABGONE CONCAGONE CONCAGO	THR THR PRO PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN GLIN GLIN GLIN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.021 40.266 39.645 40.190 39.953	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725	CONCABGONA CONCABGONE CONCABGONA CONCAGONA	THR PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN ARG ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 166 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.617 39.893 39.621 40.266 39.645 40.190 39.953 40.742	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.16 1.00 61.62 1.00 62.57 1.00 64.82 1.00 67.31	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724	CONCABG CONCABGONE CONCAGONE CONCAGO	THR PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN GLIN GLIN GLIN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.617 39.893 39.021 40.266 39.645 40.190 39.953 40.742 40.094	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.143	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 67.31 1.00 69.03	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725	CONCABGONA CONCABGONE CONCABGONA CONCAGONA	THR PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN GLIN GLIN GLIN	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 166 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.617 39.893 39.621 40.266 39.645 40.190 39.953 40.742	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539 7.591	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.65 1.00 62.45 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 69.03 1.00 69.14	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726	CONCABGONCONCONCONE	THR PRO PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN GLIN ARG ARG ARG ARG ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.617 39.893 39.021 40.266 39.645 40.190 39.953 40.742 40.094	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.143	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 67.31 1.00 69.03	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726 2727 2728	CONCABGONA CONCABGONE CONCABGONA CONCAGONA CONCAG	THR PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN ARG ARG ARG ARG ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.605 40.177 39.617 39.893 39.021 40.266 39.645 40.190 39.953 40.742 40.094 40.570	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198 52.143 51.477	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539 7.591	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.65 1.00 62.45 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 69.03 1.00 69.14	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726 2727 2728 2729	CONCABGONCONCOCCEZHI CONCABGONE CONCABGONE NA CONCABGONE NA CONCABONE NA CONCABONE N	THR PRO PRO PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN ARG ARG ARG ARG ARG ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.195 38.071 39.617 39.893 39.021 40.266 39.645 40.190 39.953 40.742 40.094 40.570 41.710 39.897	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198 52.143 51.477 50.804 51.471	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539 7.499 8.735	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 69.03 1.00 69.34 1.00 69.34	888888888888888888888888888888888888
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726 2727 2728 2729 2730	CONCABGONABGONE CONABGONE CHILLE	THR PRO PRO PRO PRO PRO PRO GLIN GLIN GLIN GLIN GLIN ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.893 39.021 40.266 39.645 40.190 39.953 40.190 39.953 40.742 40.094 40.570 41.710 39.897 38.136	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198 52.143 51.477 50.804 51.471 51.154	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539 7.499 8.735 2.333	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 69.31 1.00 69.31 1.00 69.34 1.00 69.34 1.00 69.52 1.00 59.19	**************************************
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726 2727 2728 2729 2730 2731	CONCABGONES ON CONCABGONES ON CONCABONES ON	THR PRO PRO PRO PRO PRO PRO GLIN GLIN GLIN ARG ARG ARG ARG ARG ARG ARG ARG ARG	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.893 39.617 39.893 39.621 40.266 39.645 40.190 39.953 40.742 40.94 40.570 41.710 39.897 38.136 37.647	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.492 49.287 48.635 50.501 51.11 52.525 53.029 52.198 52.143 51.477 50.804 51.615	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.556 2.535 2.777 4.204 5.237 4.204 5.237 6.539 7.499 8.735 2.333 1.303	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.7 1.00 64.82 1.00 69.31 1.00 69.34 1.00 69.34 1.00 69.34 1.00 69.34 1.00 69.34 1.00 69.39 1.00 59.19 1.00 58.60	***************************************
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2703 2704 2705 2706 2707 2708 2709 2710 2711 2712 2713 2714 2715 2716 2717 2718 2719 2720 2721 2722 2723 2724 2725 2726 2727 2728 2729 2730	CONCABGONABGONE CONABGONE CHILLE	THR PROOF PR	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	164 165 165 165 165 165 165 166 166 166 166	42.012 40.866 42.976 44.315 42.734 44.063 44.604 42.347 43.149 41.110 40.598 39.605 40.177 39.893 39.021 40.266 39.645 40.190 39.953 40.190 39.953 40.742 40.094 40.570 41.710 39.897 38.136	44.766 44.658 44.055 45.605 45.608 44.236 47.002 47.698 47.395 48.709 48.590 47.945 47.942 47.448 48.492 49.287 48.635 50.501 51.111 52.525 53.029 52.198 52.143 51.477 50.804 51.471 51.154	-1.642 -1.555 -0.770 -0.647 0.322 1.078 0.822 -0.163 -0.790 0.126 -0.250 -1.410 -2.661 -3.819 -3.697 -4.954 0.970 1.550 1.366 2.535 2.777 4.204 5.227 6.539 7.499 8.735 2.333	1.00 57.80 1.00 57.08 1.00 58.98 1.00 59.54 1.00 60.52 1.00 60.33 1.00 60.42 1.00 61.65 1.00 61.24 1.00 62.45 1.00 63.32 1.00 65.46 1.00 69.00 1.00 71.19 1.00 72.48 1.00 72.65 1.00 62.65 1.00 62.65 1.00 62.65 1.00 62.57 1.00 64.82 1.00 69.31 1.00 69.31 1.00 69.34 1.00 69.34 1.00 69.52 1.00 59.19	**************************************

ATOM	2734	С	GLY E	168	35.466	49.200	3.191	1.00 55.42	В
			GLY E		34.306	48.924	3.495	1.00 55.98	В
ATOM	2735	0							
MOTA	2736	N		3 169	36.350	48.280	2.814	1.00 53.44	В
ATOM	2737	CA	ASP E	169	35.979	46.871	2.757	1.00 51.76	В
ATOM	2738	CB	ASP E	169	36.841	46.115	1.740	1.00 50.49	В
ATOM	2739	CG	ASP E	3 169	36.428	46.392	0.311	1.00 50.57	В
ATOM	2740	OD1	ASP E		35.207	46.479	0.060	1.00 49.92	В
							-0.559	1.00 49.84	В
MOTA	2741	OD2		3 169	37.318	46.507			
MOTA	2742	C	ASP E	3 169	36.083	46.181	4.110	1.00 49.36	В
ATOM	2743	0	ASP E	3 169	37.066	46.343	4.836	1.00 48.92	В
ATOM	2744	N	VAL E	3 170	35.047	45.418	4.436	1.00 47.48	В
ATOM	2745	CA	VAL F		34.981	44.667	5.680	1.00 45.10	В
					33.800	45.130	6.543	1.00 45.86	В
ATOM	2746	CB	VAL E						
ATOM	2747	CG1	VAL I		33.702	44.268	7.795	1.00 46.26	B
MOTA	2748	CG2	VAL I	3 170	33.974	46.598	6.906	1.00 46.23	В
ATOM	2749	C	VAL E	3 170	34.787	43.191	5.342	1.00 43.62	В
ATOM	2750	0	VAL I	3 170	33.774	42.807	4.762	1.00 42.86	В
ATOM	2751	N	TYR F		35.762	42.367	5.704	1.00 41.69	В
								1.00 38.95	В
ATOM	2752	CA	TYR I		35.694	40.935	5.425		
MOTA	2753	CB	TYR I	3 171	37.044	40.455	4.899	1.00 37.52	В
ATOM	2754	CG	TYR I	3 171	37.405	41.031	3.553	1.00 38.12	В
ATOM	2755	CD1	TYR I	3 171	37.023	40.391	2.376	1.00 37.52	В
ATOM	2756	CE1	TYR I		37.342	40.923	1.131	1.00 38.06	В
					38.118	42.224	3.454	1.00 37.54	В
MOTA	2757	CD2	TYR I						
MOTA	2758	CE2	TYR I	3 171	38.442	42.767	2.216	1.00 38.45	B
MOTA	2759	CZ	TYR I	3 171	38.052	42.110	1.056	1.00 39.25	В
ATOM	2760	OH	TYR I	3 171	38.372	42.641	-0.172	1.00 38.84	В
ATOM	2761	С	TYR I	3 171	35.314	40.139	6.671	1.00 37.46	В
		o		3 171	35.791	40.428	7.773	1.00 34.85	В
ATOM	2762							1.00 35.06	В
ATOM	2763	N	THR I		34.452	39.140	6.501		
MOTA	2764	CA	THR I	3 172	34.049	38.328	7.638	1.00 35.81	В
ATOM	2765	CB	THR 1	3 172	32.589	38.622	8.064	1.00 38.37	В
ATOM	2766	OG1	THR 1	3 172	31.688	38.177	7.043	1.00 42.02	В
ATOM	2767	CG2		3 172	32.390	40.119	8.292	1.00 39.83	В
					34.182	36.830	7.406	1.00 33.71	В
MOTA	2768	C		3 172					
MOTA	2769	0		B 172	33.953	36.335	6.300	1.00 32.99	B -
ATOM	2770	N	CYS :	B 173	34.578	36.123	8.463	1.00 32.09	В
ATOM	2771	CA	CYS I	B 173	34.714	34.670	8.438	1.00 31.08	В
ATOM	2772	C	CYS	B 17 3	33.497	34.183	9.200	1.00 30.92	В
ATOM	2773	0	CYS		33.240		10.326	1.00 32.70	В
							9.155	1.00 31.48	В
MOTA	2774	CB		B 173	35.988	_			
ATOM	2775	SG	CYS :	B 173	36.338		8.983	1.00 31.85	В
ATOM	2776	N	HIS :	B 174	32.748	33.288	8.578	1.00 30.26	В
ATOM	2777	CA	HIS :	B 174	31.524	32.754	9.152	1.00 29.72	В
ATOM	2778	CB	HIS :	B 174	30.401	32.977	8.128	1.00 30.80	В
	2779	CG		B 174	29.030		8.615	1.00 32.90	В
MOTA							9.058	1.00 33.11	В
MOTA	2780	CD2		B 174	28.016				
MOTA	2781	ND1	HIS	B 174	28.551		8.621	1.00 34.85	В
ATOM	2782	CE1	HIS	B 174	27.299	31.332	9.044	1.00 37.21	В
MOTA	2783	NE2	HIS	B 174	26.950	32.577	9.316	1.00 34.95	В
ATOM	2784	C	HIS	B 174	31.751	31.271	9.449	1.00 28.49	В
ATOM	2785	Ō		B 174	32.080	30.494	8.554	1.00 27.69	В
						30.888	10.710	1.00 27.48	В
ATOM	2786	N		B 175	31.584		11.121	1.00 27.40	В
ATOM	2787	CA		B 175	31.810	29.508			
MOTA	2788	CB	VAL	B 175	32.988	29.418	12.126	1.00 25.31	B
MOTA	2789	CG1	. VAL	B 175	33.147	27.982	12.629	1.00 21.10	В
ATOM	2790	CG2	VAL	B 175	34.271	29.896	11.462	1.00 22.12	В
ATOM	2791	C	VAT	B 175	30.606	28.821	11.748	1.00 26.58	В
		Ō		B 175	30.004	29.328	12.694	1.00 27.01	В
ATOM	2792						11.212	1.00 27.17	В
MOTA	2793	N		B 176	30.274	27.652			
MOTA	2794	CA	GLU	B 176	29.168	26.846	11.712	1.00 28.51	В
ATOM	2795	CB	GLU	B 176	28.166	26.573	10.588	1.00 32.35	В
ATOM	2796	CG	GLU	B 176	27.454	27.827	10.082	1.00 38.87	В
MOTA	2797	CD		B 176	26.776	27.616	8.735	1.00 42.45	В
						26.684	8.618	1.00 43.07	В
ATOM	2798	OE1		B 176	25.947				
MOTA	2799	OE2		B 176	27.075	28.386	7.794	1.00 42.94	В
MOTA	2800	C	GLU	B 176	29.750	25.536	12.235	1.00 27.34	В
ATOM	2801	0	GLU	B 176	30.576	24.900	11.574	1.00 26.12	В
MOTA	2802	N	HIS	B 177	29.308	25.134	13.420	1.00 26.08	В
ATOM	2803	CA		B 177	29.800	23.921	14.049	1.00 26.30	В
						24.244	14.738	1.00 24.58	B
MOTA	2804	CB		B 177	31.132	_1			
MOTA	2805	CG		B 177	31.759	23.076	15.422	1.00 22.32	В
ATOM	2806	CD2		B 177	32.646	22.156	14.977	1.00 21.05	B
ATOM	2807	ND	L HIS	B 177	31.437	22.711	16.710	1.00 21.01	В

MOTA	2808	CE1	HIS F	В 177	32.097	21.613	17.030	1.00 23.72	В
ATOM	2809	NE2		B 177	32.838	21.255	15.995 15.057	1.00 23.87 1.00 27.87	B B
ATOM ATOM	2810 2811	С О		B 177 B 177	28.762 28.059	23.413 24.205	15.672	1.00 27.87	В
ATOM	2812	И		B 178	28.654	22.085	15.237	1.00 29.57	В
ATOM	2813	CD		B 178	29.365	21.025	14.501	1.00 28.96	В
ATOM	2814	CA	PRO I	B 178	27.687	21.497	16.175	1.00 31.71	В
ATOM	2815	CB		B 178	28.062	20.019	16.166	1.00 30.49	B B
ATOM	2816	CG		B 178	28.503 27.649	19.810 22.071	14.769 17.595	1.00 30.01 1.00 33.29	В
ATOM ATOM	2817 2818	С О		B 178 B 178	26.619	22.020	18.256	1.00 35.00	В
ATOM	2819	N		B 179	28.762	22.615	18.067	1.00 34.96	В
ATOM	2820	CA	SER 3	B 179	28.813	23.168	19.418	1.00 36.85	В
ATOM	2821	CB		B 179	30.261	23.228	19.896	1.00 35.35	В
ATOM	2822	OG ~		B 179	31.023	24.053 24.564	19.034 19.522	1.00 35.14 1.00 38.40	B B
ATOM	2823 2824	С О		B 179 B 179	28.206 27.953	25.056	20.619	1.00 37.27	В
ATOM ATOM	2825	И		B 180	27.971	25.192	18.377	1.00 40.10	В
ATOM	2826	CA		B 180	27.434	26.545	18.340	1.00 41.36	В
MOTA	2827	CB	LEU :	B 180	28.162	27.352	17.269	1.00 39.74	В
MOTA	2828	CG		B 180	29.677	27.432	17.422	1.00 39.93	В
ATOM	2829	CD1		B 180	30.286 30.021	28.013 28.279	16.157 18.636	1.00 39.41 1.00 39.61	B B
MOTA ATOM	2830 2831	CD2 C		B 180 B 180	25.944	26.633	18.078	1.00 43.85	В
ATOM	2832	0		B 180	25.449	26.125	17.072	1.00 44.25	В
MOTA	2833	N	GLN		25.230	27.289	18.984	1.00 47.20	В
ATOM	2834	CA	\mathtt{GLN}		23.794	27.475	18.814	1.00 49.93	В
ATOM	2835	CB	GLN		23.158	27.956	20.121	1.00 52.00 1.00 56.40	B B
ATOM	2836	CG	GLN GLN	B 181 B 181	23.873 23.263	29.134 29.538	20.758 22.084	1.00 59.03	В
ATOM ATOM	2837 2838	CD OE1		B 181	22.087	29.908	22.153	1.00 60.55	B
ATOM	2839	NE2		B 181	24.059	29.468	23.149	1.00 58.44	B
ATOM	2840	C	${ t GLN}$	B 181	23.635	28.522	17.715	1.00 49.23	В _
ATOM	2841	0		B 181	22.712	28.465	16.906	1.00 49.91	В
ATOM	2842	N	SER		24.560 24.555	29.474 30.523	17.688 16.679	1.00 48.48 1.00 47.89	B B
ATOM ATOM	2843 2844	CA CB	SER SER	B 182 B 182	24.333	31.879	17.314	1.00 48.68	В
ATOM	2845	OG	SER		25.211	32.223	18.286	1.00 50.58	В
MOTA	2846	С	SER	B 182	25.938	30.550	16.038	1.00 45.93	В
MOTA	2847	0	SER		26.945	30.354	16.714	1.00 45.13	В
MOTA	2848	N			26.004	30.783 31.096	14.721 13.784	1.00 45.12 1.00 44.93	B B
MOTA	2849 2850	CD CA		B 183 B 183	24.911 27.302	30.819	14.042	1.00 43.29	В
MOTA MOTA	2851	CB		B 183	26.923	31.070	12.581	1.00 43.70	В
MOTA	2852	CG	PRO	B 183	25.642	31.833	12.688	1.00 44.70	В
ATOM	2853	C	PRO	B 183	28.254	31.876	14.593	1.00 40.67	В
MOTA	2854	0		B 183	27.828	32.851	15.209	1.00 40.46 1.00 37.76	B B
ATOM	2855	N		B 184 B 184	29.547 30.550	31.664 32.607	14.382 14.842	1.00 37.78	В
ATOM ATOM	2856 2857	CA CB		B 184	31.759	31.889	15.468	1.00 35.92	В
ATOM	2858	CG2		B 184	32.907	32.867	15.657	1.00 35.57	В
ATOM	2859	CGI	L ILE	B 184	31.362	31.270	16.806	1.00 36.74	В
MOTA	2860	CD		B 184	32.475	30.477	17.458	1.00 36.59	В
MOTA	2861	C	ILE	B 184	31.040	33.453 32.932	13.680 12.630	1.00 34.88 1.00 35.06	B B
MOTA	2862 2863	N	ILE THR		31.412 31.043	34.764	13.876	1.00 33.00	В
MOTA MOTA	2864	CA	THR		31.500	35.675	12.845	1.00 34.32	В
ATOM	2865	CB	THR		30.356	36.592	12.341	1.00 35.40	В
MOTA	2866	OG:	1 THR	B 185	29.770	37.285	13.450	1.00 37.01	В
ATOM	2867	CG:			29.286	35.774	11.631	1.00 35.73 1.00 33.38	B B
MOTA	2868	C		B 185	32.622 32.559	36.548 37.050	13.375 14.494	1.00 33.38 1.00 32.86	В
ATOM ATOM	2869 2870	N	THR.	B 185 B 186	33.652		12.560	1.00 32.69	В
ATOM	2871	CA			34.791	37.538	12.911	1.00 33.21	В
MOTA	2872	CB	VAL		36.041	36.683		1.00 33.39	В
ATOM	2873	CG			37.212			1.00 33.93	В
ATOM	2874	CG:			35.766	35.674 38.454		1.00 33.67 1.00 34.68	B B
ATOM	2875 2876	С О	VAL VAL		35.023 35.060			1.00 34.68	В
MOTA MOTA	2876 2877	N	GLU		35.000			1.00 36.30	В
ATOM	2878	CA			35.373			1.00 38.96	В
ATOM	2879	CB			34.484			1.00 40.90	В
MOTA	2880	CG			33.008			1.00 46.09	В
ATOM	2881	CD	GLU	B 187	32.146	42.876	11.421	1.00 48.81	В

ATOM	2882	OE1	GLU E	3	187	30.909	42.73	9	11.545	1.00	51.77	В
ATOM	2883	OE2	GLU F	3 :	187	32.701	43.99	7	11.363	1.00	49.79	В
ATOM	2884	C	GLU E		187	36.816	41.17		10.784	1.00	39.59	В
						37.637	40.99		11.684		39.84	В
MOTA	2885	0	GLU E		187							В
ATOM	2886	N	TRP F		188	37.113	41.76		9.635		39.59	
MOTA	2887	CA	TRP E	3	188	38.430	42.30	2	9.360		40.86	В
MOTA	2888	CB	TRP F	3	188	39.339	41.25	2	8.736	1.00	38.70	B
ATOM	2889	CG	TRP I	3	188	40.769	41.70	4	8.693	1.00	37.82	В
ATOM	2890	CD2	TRP F		188	41.421	42.38	13	7.615	1.00	36.62	В
							42.64		8.023		36.31	В
ATOM	2891	CE2	TRP I		188	42.748						
ATOM	2892	CE3	TRP I	3	188	41.013	42.79		6.340		36.14	B
ATOM	2893	CD1	TRP I	3	188	41.698	41.58	33	9.686	1.00	37.31	В
ATOM	2894	NE1	TRP I	3	188	42.890	42.14	1	9.291	1.00	37.27	В
ATOM	2895	CZ2	TRP I	3	188	43.673	43.29	96	7.204	1.00	37.17	В
		CZ3			188	41.932	43.45		5.522	1.00	38.70	В
ATOM	2896						43.69		5.960	1.00	37.13	В
ATOM	2897	CH2			188	43.249						
MOTA	2898	C	TRP 1	3	188	38.258	43.45		8.383		42.97	В
MOTA	2899	O	TRP I	3	188	37.946	43.24	f O	7.211	1.00	42.37	B
ATOM	2900	N	ARG I	3	189	38.442	44.67	78	8.864	1.00	46.69	В
ATOM	2901	CA	ARG I	В	1.89	38.303	45.84	12	7.999	1.00	50.32	В
	2902	CB			189	37.731	47.04	ın	8.776	1.00	52.18	В
ATOM	_					38.615	47.59		9.893	1.00	56.00	В
ATOM	2903	CG			189							В
ATOM	2904	CD	ARG I	В	189	38.234	47.04		11.270	1.00	59.95	
MOTA	2905	NE	ARG :	В	189	38.639	45.65	50	11.479	1.00		В
ATOM	2906	CZ	ARG I	В	189	39.903	45.23	36	11.559	1.00	64.33	В
MOTA	2907	NH1	ARG :	В	189	40.899	46.10)5	11.447	1.00	65.45	В
ATOM	2908	NH2			189	40.172	43.95	5.1	11.760	1.00	64.46	В
						39.664	46.19		7.412	1.00	50.56	В
MOTA	2909	C			189							В
ATOM	2910	0	ARG :		189	40.680	46.1		8.100	1.00	50.34	
ATOM	2911	N	ALA	В	190	39.684	46.55	54	6.135	1.00	52.30	В
ATOM	2912	CA	ALA	В	190	40.933	46.91	L1	5.476	1.00	54.16	В
ATOM	2913	CB	ALA	В	190	40.846	46.59	92	3.987	1.00	55.33	В
ATOM	2914	C	ALA			41.238	48.39	92	5.679	1.00	55.19	В
			ALA			40.300	49.14		6.023		54.90	В
ATOM	2915	0							5.481		56.19	B
ATOM	2916	OXT				42.408	48.78					
MOTA	2917	C	LEU	C	1.	32.073	1.03		33.225	1.00		C
MOTA	2918	0	LEU	C	1	33.091	1.60	07	33.619		35.87	C
ATOM	2919	N	LEU	C	1	29.791	1.90	06	32.702	1.00	36.17	C
ATOM	2920	CA	LEU	C	1	30.699	1.40	09	33.777	1.00	34.35	C
ATOM	2921	N	GLN		2	32.105	0.0	72	32.307	1.00	34.64	C
			GLN		2	33.374	-0.3		31.737	1.00	34.20	C
MOTA	2922	CA					-0.8		30.294	1.00		C
MOTA	2923	C	GLN		2	33.250						C
ATOM	2924	0	GLN	C	2	32.373	-1.6		29.955	1.00		
MOTA	2925	И	PRO	C	3	34.130	-0.3	29	29.418	1.00		C
ATOM	2926	CD	PRO	C	3	35.226	0.63	32	29.639	1.00	33.81	C
MOTA	2927	CA	PRO	C	3	34.064	-0.7	42	28.015	1.00	34.77	C
MOTA	2928	CB	PRO		3	35.027	0.2	22	27.329	1.00	34.33	C
					3	36.070			28.393	1.00		C
MOTA	2929	CG	PRO						27.890	1.00		Ċ
MOTA	2930	C	PRO		3	34.508						C
MOTA	2931	0	PRO	C	3	35.435			28.579	1.00		
ATOM	2932	N	PHE	C	4	33.837	-2.9	47	27.024	1.00	31.97	C
MOTA	2933	CA	PHE	C	4	34.173	-4.3	55	26.812	1.00	32.26	С
MOTA	2934	CB	PHE	C	4	32.897	-5.1	93	26.632	1.00	34.22	C
ATOM	2935	CG	PHE		4	32.006	-5.2	35	27.852	1.00	37.02	С
	2936	CD			4	32.481			29.103	1.00	38.53	C
ATOM									27.756	1.00		C
MOTA	2937	CD2			4	30.701						C
MOTA	2938	CE	L PHE	C	4	31.673			30.248		40.80	
ATOM	2939	CE	PHE	C	4	29.878			28.891	1.00		C
ATOM	2940	CZ	PHE	C	4	30.369	-5.4	21	30.142	1.00	40.74	C
ATOM	2941	C	PHE	C	4	35.052	-4.4	83	25.571	1.00	29.17	C
ATOM	2942	0	PHE	\mathbf{C}	4	34.655	-4.0	72	24.482	1.00	30.93	C
ATOM	2943	N	PRO		5	36.257		59	25.715	1.00	26.63	C
						36.936			26.974		24.97	C
MOTA	2944	CD	PRO		5							Ċ
MOTA	2945	CA	PRO			37.168			24.577	1.00		
MOTA	2946	CB	PRO	C	5	38.527	_		25.227	1.00		C
ATOM	2947	CG	PRO	C	5	38.335			26.504	1.00		C
ATOM	2948	C	PRO	C	5	37.043	-6.5	69	23.887	1.00	22.95	C
ATOM	2949	0	PRO	C	5	36.403	-7.4	75	24.404	1.00	22.96	C
ATOM	2950	N	GLN			37.666	_	96	22.719	1.00	23.53	C
	2951	CA				37.659	_		21.967	1.00		C
ATOM						37.506	_		20.475	1.00		C
MOTA	2952	CB	GLN							1.00		C
MOTA	2953	CG	GLN			36.170			20.063			
MOTA	2954	CD				36.074			18.557	1.00		C
MOTA	2955	OE	1 GLN	C	6	36.483	-7.7	760	17.773	1.00	23.94	C
								_				

MOTA	2956	NE2	GLN	C	6	35.525	-5.766	18.149	1.00 20.70	C
MOTA	2957	C	GLN	C	6	38.996	-8.637	22.204	1.00 20.71	C
ATOM	2958	0	GLN	C	6	40.046	-8.008	22.105	1.00 19.85	C
ATOM	2959	N	PRO	C	7	38.974	-9.932	22.548	1.00 21.37	C
ATOM	2960	CD	PRO		7	37.810	-10.710	23.017	1.00 21.21	C
ATOM	2961	CA	PRO		7	40.215	-10.673	22.790	1.00 21.62	С
		CB	PRO		7		-11.730	23.795	1.00 21.96	Ċ
ATOM	2962							23.755	1.00 20.65	C
ATOM	2963	CG	PRO		7		-12.085			
ATOM	2964	C	PRO		7		-11.316	21.511	1.00 24.05	C
ATOM	2965	0	PRO	С	7		-11.577	20.588	1.00 22.84	C
MOTA	2966	N	GLU	C	8	42.051	-11.550	21.448	1.00 26.22	C
MOTA	2967	CA	GLU	C	8	42.631	-12.215	20.292	1.00 27.00	C
MOTA	2968	CB	GLU	C	8	44.038	-11.687	19.988	1.00 27.94	С
ATOM	2969	CG	GLU	C	8	44.803	-12.494	18.915	1.00 28.38	C
ATOM	2970	CD	GLU	C	8	44.043	-12.649	17.589	1.00 31.32	C
ATOM	2971	OE1	GLU		8	42.980	-13.309	17.564	1.00 31.69	С
ATOM	2972	OE2	GLU		8		-12.112	16.563	1.00 29.86	C
		C	GLU		8	42.678		20.676	1.00 28.48	C
ATOM	2973				8		-14.029	21.829	1.00 28.74	C
ATOM	2974	0	GLU							C
ATOM	2975	N	LEU		9		-14.571	19.721		
MOTA	2976	ÇA	LEU		9		-15.998	20.002	1.00 31.21	C
ATOM	2977	CB	LEU	C	9	41.313	-16.688	19.183	1.00 32.12	C
MOTA	2978	CG	\mathbf{LEU}	C	9	39.918	-16.072	19.302	1.00 33.78	C
ATOM	2979	CD1	LEU	C	9	38.941	-16.866	18.457	1.00 35.00	C
ATOM	2980	CD2	LEU	C	9	39.481	-16.061	20.761	1.00 35.59	C
ATOM	2981	C	LEU	C	9	43.748	-16.641	19.712	1.00 31.83	C
ATOM	2982	0	LEU	С	9	44.342	-16.415	18.658	1.00 30.94	C
ATOM	2983	N		C	10	44.256	-17.442	20.657	1.00 33.31	C
ATOM	2984	CD	PRO		10		-17.661	22.032	1.00 33.12	С
	2985	CA			10	45.545		20.439	1.00 36.08	C
ATOM							-18.590	21.836	1.00 36.62	Ċ
ATOM	2986	CB	PRO		10				1.00 35.26	C
MOTA	2987	CG	PRO		1.0	44.598		22.476		
ATOM	2988	C	PRO		10	45.428		19.430	1.00 37.51	C
MOTA	2989	0	PRO	C	10	44.495		19.491	1.00 39.49	C
ATOM	2990	N	TYR	C	11	46.365	-19.269	18.488	1.00 38.68	C
ATOM	2991	CA	TYR	C	11.	46.392	-20.305	17.463	1.00 40.24	C
ATOM	2992	С	TYR	C	11	47.834	-20.782	17.290	1.00 42.03	C
ATOM	2993	0	TYR	C	11	48.121	-21.967	17.586	1.00 42.72	C
ATOM	2994	OXT	TYR	C	11	48.665	-19.949	16.870	1.00 42.75	C
ATOM	2995	CB	VAL		2	76.722	40.050	4.030	1.00 35.81	D
ATOM	2996	CG1	VAL		2	77.537	40.465	2.823	1.00 36.64	D
ATOM	2997	CG2	VAL		2	76.313	38.577	3.893	1.00 37.71	D
		C	VAL		2	76.622	40.298	<i>c</i> ====	1.00 31.61	D
ATOM	2998					75.696	39.494	6.653	1.00 31.96	D
ATOM	2999	0	VAL		2				1.00 32.12	D
ATOM	3000	N	VAL		2	78.625	39.207	5.418		
ATOM	3001	CA	VAL		2	77.560	40.255	5.317	1.00 33.74	D
MOTA	3002	N	ALA	D	3	76.864	41.246	7.441	1.00 29.52	D
MOTA	3003	CA	ALA	D	3	76.053	41.379	8.653	1.00 27.92	D
MOTA	3004	CB	ALA	D	3	76.480	40.321	9.684	1.00 27.11	D
MOTA	3005	C	ALA	D	3	76.128	42.767	9.286	1.00 25.71	D
ATOM	3006	0	ALA	D	3	77.050	43.540	9.016	1.00 23.11	D
ATOM	3007	N	ASP	D	4	75.152	43.070	10.137	1.00 24.26	D
MOTA	3008	CA	ASP	D	4	75.109	44.354	10.825	1.00 24.77	D
ATOM	3009	CB	ASP		4	73.774	44.533	11.555	1.00 25.88	D
MOTA	3010	CG	ASP		4	72.595		10.611	1.00 26.24	D
ATOM	3011		ASP		4	71.449		11.080	1.00 24.74	D
						72.811		9.416	1.00 28.25	D
ATOM	3012		ASP		4			11.857	1.00 25.25	D
ATOM	3013	C	ASP		4	76.230				
MOTA	3014	0	ASP		4	76.882		12.027	1.00 26.40	D
ATOM	3015	N	HIS	D	5	76.440		12.549	1.00 24.52	D
ATOM	3016	CA	HIS	D	5	77.469		13.582	1.00 24.25	D
MOTA	3017	CB	HIS	D	5	76.836	43.302	14.972	1.00 23.42	D
MOTA	3018	CG	HIS	D	5	76.138	44.599	15.231	1.00 26.12	D
MOTA	3019	CD2	HIS	D	5	76.567	45.879	15.126	1.00 26.16	D
ATOM	3020		HIS		5	74.830	44.667	15.657	1.00 25.67	D
ATOM	3021		HIS		5	74.481		15.799	1.00 26.53	D
ATOM	3022	NE2			5	75.516		15.484	1.00 25.96	D
ATOM	3022	C	HIS		5	78.241		13.492	1.00 22.88	D
					5 5	77.657	_	13.452	1.00 22.31	D
ATOM	3024	O	HIS					13.691	1.00 20.27	D
ATOM	3025	N	VAL		6	79.552				D
ATOM	3026	CA	VAL		6	80.421		13.657		
MOTA	3027	CB	VAL		6 `	81.419		12.486	1.00 20.45	D
MOTA	3028	CG1			6	82.357		12.564	1.00 19.85	D
MOTA	3029	CG2	VAL	D	6	80.674	40.869	11.161	1.00 25.29	D

ATOM	3030	С	VAL	D	6	81.223	40.792	14.944	1.00 18.77	D
MOTA	3031	0	VAL	D	6	81.767	41.812	15.352	1.00 17.70	D
MOTA	3032	N	ALA		7	81.304	39.626	15.575	1.00 18.23	D
MOTA	3033	CA	ALA		7	82.046	39.489	16.821	1.00 18.01	Ď
ATOM	3034	CB	ALA		7	81.080	39.452	18.006	1.00 17.61	D
ATOM	3035	C	ALA		7	82.899	38.239	16.838	1.00 17.37 1.00 19.56	D D
ATOM	3036	N	ALA SER		7 8	82.568 84.008	37.242 38.306	16.208 17.562	1.00 19.56	D D
ATOM ATOM	3037 3038	CA	SER		8	84.892	37.158	17.712	1.00 17.07	D
MOTA	3038	CB	SER		8	86.297	37.455	17.202	1.00 12.56	D
ATOM	3040	OG	SER		8	86.324	37.492	15.789	1.00 18.97	D
ATOM	3041	C	SER		8	84.932	36.904	19.201	1.00 16.39	D
ATOM	3042	0	SER		8	85.613	37.614	19.951	1.00 15.61	D
ATOM	3043	N	TYR		9	84.144	35.930	19.637	1.00 17.58	D
ATOM	3044	CA	TYR	D	9	84.096	35.587	21.044	1.00 18.51	D
ATOM	3045	CB	TYR	D	9	82.698	35.133	21.444	1.00 17.92	D
ATOM	3046	CG	TYR	D	9	81.730	36.290	21.362	1.00 17.41	Ð
ATOM	3047	CD1	TYR		9	82.056	37.523	21.928	1.00 16.27	D
ATOM	3048	CE1	TYR		9	81.208	38.603	21.840	1.00 15.18	D
MOTA	3049	CD2	TYR		9	80.515	36.169	20.701	1.00 17.05	D
ATOM	3050	CE2	TYR		9	79.649	37.252	20.608	1.00 18.01 1.00 16.67	D D
ATOM	3051	CZ	TYR		9 9	80.005 79.157	38.466 39.543	21.181 21.104	1.00 20.30	D
ATOM	3052	OH C	TYR TYR		9	85.120	34.508	21.104	1.00 20.30	D
ATOM ATOM	3053 3054	0	TYR		9	84.856	33.323	21.337	1.00 17.21	D
ATOM	305 4	N	GLY		10	86.321	34.989	20.843	1.00 22.61	D
ATOM	3056	CA	GLY		10	87.478	34.160	20.836	1.00 20.96	D
ATOM	3057	C	GLY		10	88.358	34.354	19.624	1.00 18.79	D
ATOM	3058	0	GLY		10	88.170	33.693	18.618	1.00 16.79	D
ATOM	3059	N	VAL		11	89.275	35.307	19.683	1.00 17.75	D
ATOM	3060	CA	VAL	D	11	90.256	35.394	18.616	1.00 16.92	D
ATOM	3061	CB	VAL	D	11	90.666	36.829	18.242	1.00 17.76	D
MOTA	3062	CG1	VAL	D	11	91.873	36.778	17.313	1.00 15.46	D
ATOM	3063	CG2	VAL	D	11	89.522	37.544	17.544	1.00 13.00	D
MOTA	3064	C	LAV		11	91.391	34.728	19.395	1.00 17.46	D
ATOM	3065	0	VAL		11	91.865	35.266	20.405	1.00 18.93	D
ATOM	3066	N	ASN		12	91.773	33.531	18.973	1.00 17.46 1.00 18.01	D D
ATOM	3067	CA	ASN		12	92.831	32.779 31.360	19.644 19.969	1.00 16.68	D
MOTA	3068	CB	ASN		12 12	92.339 91.179	31.356	20.955	1.00 16.27	D
MOTA	3069 3070	CG OD1	ASN ASN		1.2	91.346	30.989	22.115	1.00 14.97	D
ATOM ATOM	3070	ND2			12	90.000	31.779	20.497	1.00 14.97	D
ATOM	3072	C	ASN		12	94.061	32.699	18.759	1.00 18.74	D
ATOM	3073	0	ASN		12	93.963	32.373	17.578	1.00 19.66	D
ATOM	3074	N	LEU		13	95.221	32.969	19.344	1.00 20.75	D
ATOM	3075	CA	LEU	D	13	96.471	32.949	18.600	1.00 22.59	D
MOTA	3076	CB	LEU	D	13	96.841	34.387	18.234	1.00 24.32	D
ATOM	3077	CG	LEU	D	13	98.215	34.672	17.632	1.00 25.29	D
ATOM	3078		LEU		13	98.355	33.966	16.289	1.00 24.58	D
MOTA	3079		LEU		13	98.380	36.177	17.475	1.00 23.52	D
ATOM	3080					97.646	32.290	19.330	1.00 22.44 1.00 24.67	D D
MOTA	3081	0	LEU		13	97.900 98.350	32.578 31.397	20.494 18.641	1.00 24.67	D
ATOM	3082 3083	N CA	TYR TYR		14 14	99.535	30.740	19.196	1.00 25.57	D
ATOM ATOM	3084	CB	TYR		14	99.223	29.360	19.765	1.00 26.53	D
ATOM	3085	CG	TYR		14	100.445	28.712	20.383	1.00 28.87	D
ATOM	3086	CD1			14	100.872	29.057	21.668	1.00 28.57	α
ATOM	3087	CE1			14	102.032	28.500	22.218	1.00 27.29	D
ATOM	3088	CD2		D	14	101.209	27.793	19.664	1.00 29.65	D
ATOM	3089	CE2	TYR	D	14	102.369	27.235	20.204	1.00 26.94	D
MOTA	3090	CZ	TYR	D	14	102.773	27.592	21.477	1.00 27.22	D
ATOM	3091	OH	TYR	D	14	103.914	27.039	22.008	1.00 29.69	D
MOTA	3092	C	TYR		14	100.553	30.574	18.074	1.00 26.73	D
MOTA	3093	0	TYR		14	100.210	30.128	16.980	1.00 27.22	D
ATOM	3094	N	GLN		15	101.800	30.945	18.338	1.00 26.92	D D
MOTA	3095	CA	GLN		15	102.847	30.820	17.332 16.710	1.00 27.70 1.00 27.39	D
MOTA	3096	CB	GLN		15 15	103.164 103.534	32.179 33.251	17.704	1.00 27.39	D
ATOM ATOM	3097 3098	CG CD	GLN GLN		15 15	103.806	34.590	17.704	1.00 27.78	D
ATOM	3098	OE1			15	103.723	35.638	17.685	1.00 31.07	D
ATOM	3100	NE2			15	104.142	34.562	15.763	1.00 25.83	D
ATOM	3101	C	GLN		15	104.097	30.222	17.952	1.00 28.40	D
ATOM	3102	ō	GLN		15	104.368	30.416	19.141	1.00 28.81	D
ATOM	3103	N	SER	D	16	104.852	29.488	17.143	1.00 27.95	D

ATOM	3104	CA	SER	D	16	106.070	28.834	17.611	1.00 28.04	D
ATOM	3105	CB	SER		16	106.613	27.887	16.534	1.00 25.04	D
ATOM	3106	OG	SER		16	106.879	28.581	15.330	1.00 26.28	D
ATOM	3107	C	SER		16	107.155	29.824	18.024	1.00 27.77	D
ATOM	3108	0	SER		16	107.922	29.558	18.946	1.00 26.81	D
ATOM	3109	N	TYR		17	107.221	30.965	17.351	1.00 29.70	D
ATOM	3110	CA	TYR		17	108.228	31.953	17.694	1.00 32.41	D
ATOM	3111	CB	TYR		17	108.248	33.086	16.672	1.00 35.15	D
ATOM	3112	CG	TYR		17	109.440	33.986	16.864	1.00 40.80	D
ATOM	3113	CD1		D	17	110.719	33.556	16.508	1.00 43.28	D
ATOM	3114	CE1	TYR	_	17	111.836	34.345	16.743	1.00 44.62	D
ATOM	3115	CD2	TYR		17	109.308	35.235	17.460	1.00 40.97	D
ATOM	3116	CE2	TYR		17	110.419	36.032	17.702	1.00 44.83	D
ATOM	3117	CZ	TYR		17	111.679	35.580	17.341	1.00 45.74	D
ATOM	3118	OH	TYR		17	112.788	36.353	17.590	1.00 49.39	D
ATOM	3119	C	TYR	D	17	107.954	32.525	19.084	1.00 33.13	D
ATOM	3120	0	TYR	Ð	17	106.888	33.092	19.332	1.00 32.77	D
ATOM	3121	N	GLY	D	18	108.930	32.383	19.981	1.00 32.74	D
ATOM	3122	CA	GLY		1.8	108.780	32.867	21.341	1.00 31.76	D
ATOM	3123	C	GLY	D	18	108.958	31.716	22.311	1.00 32.63	D
ATOM	3124	0	GLY	D	18	110.005	31.600	22.948	1.00 34.20	D
ATOM	3125	N	PRO	D	19	107.946	30.840	22.452	1.00 33.13	D
ATOM	3126	CD	PRO	D	19	108.029	29.606	23.256	1.00 31.73	D
ATOM	3127	CA	PRO	D	19	106.663	30.906	21.741	1.00 32.71	D
ATOM	3128	СВ	PRO	D	19	106.115	29.492	21.903	1.00 33.20	D
ATOM	3129	CG	PRO	D	19	106.591	29.128	23.280	1.00 31.76	D
ATOM	3130	C	PRO	D	19	105.768	31.948	22.406	1.00 32.52	D
MOTA	3131	0	PRO	D	19	105.970	32.282	23.568	1.00 33.11	D
MOTA	3132	N	SER	D	20	104.786	32.463	21.676	1.00 31.92	D
ATOM	3133	CA	SER	D	20	103.886	33.455	22.246	1.00 30.99	D
MOTA	3134	CB	SER	D	20	104.287	34.867	21.795	1.00 30.92	D
MOTA	3135	OG	SER	D	20	104.263	34.988	20.381	1.00 33.16	D
ATOM	3136	C	SER	D	20	102.441	33.172	21.852	1.00 30.01	D -
ATOM	3137	O	SER	D	20	102.179	32.428	20.902	1.00 29.42	D -
ATOM	3138	N	GLY	D	21	101.512	33.763	22.598	1.00 27.60	D
MOTA	3139	CA	GLY	D	21	100.101	33.580	22.318	1.00 25.70	D
MOTA	3140	C	GLY		21	99.309	34.836	22.632	1.00 24.66	D
ATOM	3141	0	GLY		21	99.848	35.798	23.187	1.00 23.84	D
MOTA	3142	N	GLN		22	98.030	34.834	22.268	1.00 22.55	D
ATOM	3143	CA	GLN		22	97.149	35.974	22.527	1.00 20.16	D
MOTA	3144	CB	GLN		22	97.301	37.049	21.445	1.00 18.28	D D
MOTA	3145	CG	GLN		22	96.416	38.284	21.672	1.00 18.60 1.00 18.36	D
ATOM	3146	CD	GLN		22	96.513	39.327	20.562	1.00 19.82	D
MOTA	3147	OE1			22	97.379	40.207	20.587	1.00 17.69	D
MOTA	3148	NE2			22	95.617	39.232	19.582 22.561	1.00 17.69	D
ATOM	3149	C	GLN		22	95.699	35.517	22.301	1.00 17.26	D
MOTA	3150	0	GLN		22	95.301	34.638	23.475	1.00 17.20	D
ATOM	3151	N	TYR		23	94.926 93.507	36.097 35.785	23.592	1.00 16.21	D
ATOM	3152	CA	TYR		23	93.212	34.839	24.762	1.00 14.97	D
MOTA	3153	CB	TYR		23	91.750	34.438	24.798	1.00 14.24	D
ATOM	3154	CG	TYR		23 23	91.730	33.318	24.109	1.00 14.49	D
ATOM	3155	CD1	TYR TYR		23	89.969	33.004	24.029	1.00 14.23	D
ATOM	3156				23	90.795	35.240	25.421	1.00 13.21	D
ATOM	3157	CD2 CE2			23	89.443	34.934	25.344	1.00 13.08	D
ATOM	3158	CE2	TYR		23	89.039	33.814	24.647	1.00 12.88	D
ATOM ATOM	3159 3160	OH	TYR		23	87.710	33.471	24.566	1.00 16.44	D
ATOM	3161	C	TYR		23	92.751	37.089	23.806	1.00 15.56	D
ATOM	3162	0	TYR		23	93.014	37.817	24.763	1.00 16.57	D
MOTA	3163	N	THR		24	91.811	37.377	22.914	1.00 14.11	D
ATOM	3164	CA	THR		24	91.026	38.598	22.995	1.00 13.31	D
ATOM	3165	CB	THR		24	91.606	39.692	22.071	1.00 16.07	D
ATOM	3166	OG1			24	91.682	39.176	20.734	1.00 17.94	D
ATOM	3167	CG2			24	92.992	40.116	22.514	1.00 13.19	D
ATOM	3168	C	THR		24	89.604	38.342	22.519	1.00 12.68	D
ATOM	3169	0	THR		24	89.306	37.287	21.994	1.00 15.13	D
ATOM	3170	N	HIS		25	88.726	39.312	22.727	1.00 13.47	D
ATOM	3171	CA	HIS		25	87.360	39.224	22.229	1.00 13.83	D
ATOM	3172	CB	HIS		25	86.326	39.132	23.346	1.00 11.26	D
ATOM	3173	CG	HIS		25	86.053	37.727	23.785	1.00 14.42	D
ATOM	3174	CD2			25	86.815	36.610	23.723	1.00 12.09	D
ATOM	3175	NDI			25	84.876	37.351	24.392	1.00 15.93	D
ATOM	3176	CE1	L HIS	S D	25	84.922	36.064	24.685	1.00 14.24	D
ATOM	3177	NE	HIS	D	25	86.089	35.591	24.289	1.00 13.67	D
								30		

MOTA	3178	С	HIS	D	25	87.158	40.495	21.436	1.00 13.30	D
ATOM	3179	0	HIS	D	25	87.573	41.563	21.859	1.00 13.77	D
ATOM	3180	N	GLU	D	26	86.544	40.376	20.271	1.00 15.40	D
			GLU		26	86.318	41.540	19.434	1.00 16.53	D
ATOM	3181	CA								
ATOM	3182	CB	GLU		26	87.109	41.396	18.133	1.00 14.47	D
ATOM	3183	CG	GLU	D	26	88.627	41.460	18.277	1.00 14.81	D
ATOM	3184	CD	GLU	D	26	89.341	41.205	16.947	1.00 19.22	D
ATOM	3185	OE1	GLU	D	26	88.726	41.429	15.884	1.00 22.84	D
ATOM	3186	OE2	GLU		26	90.512	40.792	16.953	1.00 17.41	D
ATOM	3187	C	GLU		26	84.841	41.721	19.111	1.00 17.28	D
ATOM	3188	0	GLU	D	26	84.073	40.760	19.100	1.00 16.62	D
ATOM	3189	N	PHE	D	27	84.455	42.971	18.879	1.00 19.63	D
ATOM	3190	CA	PHE	D	27	83.092	43.313	18.494	1.00 19.71	D
ATOM	3191	CB		D	27	82.231	43.722	19.684	1.00 21.05	D
					27		43.816	19.348	1.00 24.29	D
ATOM	3192	CG	PHE			80.758				
ATOM	3193	CD1	PHE		27	79.971	42.668	19.278	1.00 23.22	D
ATOM	3194	CD2	PHE	D	27	80.169	45.047	19.073	1.00 22.47	D
ATOM	3195	CE1	PHE	D	27	78.617	42.744	18.940	1.00 24.89	D
ATOM	3196	CE2	PHE	D	27	78.818	45.132	18.733	1.00 24.72	D
ATOM	3197	CZ	PHE	D	27	78.041	43.980	18.667	1.00 22.80	D
		C	PHE		27	83.182	44.482	17.532	1.00 18.41	D
ATOM	3198									
ATOM	3199	0		D	27	83.700	45.545	17.879	1.00 19.21	D
MOTA	3200	N	ASP	D	28	82.680	44.272	16.321	1.00 18.46	D
ATOM	3201	CA	ASP	D	28	82.700	45.284	15.272	1.00 18.63	D
ATOM	3202	CB	ASP	D	28	81.702	46.404	15.568	1.00 19.29	D
ATOM	3203	CG		D	28	80.268	45.981	15.305	1.00 22.52	D
ATOM	3204	OD1		D	28	80.076	44.885	14.738		D
ATOM	3205	OD2	ASP	D	28	79.333	46.736	15.651	1.00 24.61	D
ATOM	3206	C	ASP	D	28	84.075	45.865	15.037	1.00 17.83	D
ATOM	3207	0	ASP	D	28	84.225	47.069	14.860	1.00 20.60	D
ATOM	3208	N	GLY	D	29	85.079	44.997	15.042	1.00 18.44	D
ATOM	3209	CA	GLY		29	86.439	45.431	14.788	1.00 19.49	D
										D
ATOM	3210	C	GLY		29	87.218	46.011	15.949	1.00 18.93	
ATOM	3211	0	GLY	D	29	88.382	46.359	15.784	1.00 19.51	D
ATOM	3212	N	ASP	D	30	86.595	46.122	17.117	1.00 17.91	D
ATOM	3213	CA	ASP	D	30	87.279	46.667	18.288	1.00 17.21	D
ATOM	3214	CB	ASP	D	30	86.499	47.858	18.831	1.00 15.85	D
ATOM	3215	CG		D	30	86.594	49.060	17.924	1.00 18.96	D
ATOM	3216	OD1	ASP		30	87.731	49.515	17.668		D
ATOM	3217	OD2	ASP	D	30	85.541	49.544	17.466	1.00 19.00	
MOTA	3218	C	ASP	D	30	87.491	45.629	19.389	1.00 17.20	D
ATOM	3219	0	ASP	D	30	86.651	44.763	19.621	1.00 15.68	D
ATOM	3220	N	GLU	D	31	88.629	45.739	20.062	1.00 18.79	D
ATOM	3221	CA	GLU		31	89.015	44.829	21.131	1.00 17.52	
MOTA	3222	CB	GLU		31	90.531	44.947	21.363	1.00 19.03	D
ATOM	3223	CG	GLU	D	31	91.074	44.215	22.579	1.00 22.08	D
ATOM	3224	CD	GLU	D	31.	92.596	44.254	22.653	1.00 25.29	D
ATOM	3225	OE1	GLU	D	31	93.198	45.159	22.041	1.00 26.54	D
ATOM	3226	OE2	GLU	D	31	93.193	43.387	23.331	1.00 25.19	D
ATOM	3227	C	GLU		31	88.248	45.109	22.421	1.00 17.80	
MOTA	3228	0	GLU		31	88.360	46.195	23.004	1.00 16.81	
MOTA	3229	N	GLN		32	87.478	44.118	22.862	1.00 15.25	
MOTA	3230	CA	GLN	D	32	86.685	44.230	24.085	1.00 15.53	D
MOTA	3231	CB	GLN	D	32	85.502	43.260	24.044	1.00 12.86	D
ATOM	3232	CG	GLN	D	32	84.391	43.680	23.101	1.00 13.72	D
ATOM	3233	CD	GLN		32	83.233	42.708	23.111	1.00 16.53	
									1.00 20.27	
ATOM	3234	OE1	GLN		32	83.407	41.526	22.838		
MOTA	3235	NE2	GLN	D	32	82.044	43.203	23.423	1.00 17.48	
ATOM	3236	C	GLN	D	32	87.528	43.956	25.329	1.00 16.00	D
ATOM	3237	0	GLN	D	32	87.356	44.603	26.366	1.00 15.18	D
ATOM	3238	N	PHE	D	33	88.423	42.981	25.222	1.00 16.17	D
ATOM	3239	CA	PHE		33	89.315	42.638	26.321	1.00 15.74	D
			PHE		33	88.520	42.083	27.515	1.00 15.40	
ATOM	3240	CB								
ATOM	3241	CG	PHE		33	87.969	40.693	27.307	1.00 15.83	
MOTA	3242	CD1	PHE	D	33	88.781	39.572	27.480	1.00 16.23	
ATOM	3243	CD2	PHE	D	33	86.625	40.503	26.977	1.00 17.27	D
ATOM	3244		PHE		33	88.262	38.282	27.332	1.00 15.79	D
ATOM	3245	CE2	PHE		33	86.088	39.218	26.827	1.00 15.20	. D
ATOM	3246	CZ	PHE		33	86.909	38.108	27.006	1.00 17.77	
ATOM	3247	C	PHE		33	90.330	41.614	25.860		
MOTA	3248	0	PHE		33	90.157	40.979	24.825	1.00 15.16	
MOTA	3249	N	TYR	D	34	91.405	41.476	26.620	1.00 15.54	
ATOM	3250	CA	TYR	D	34	92.414	40.480	26.314	1.00 16.00	D
ATOM	3251	CB	TYR		34	93.649	41.124	25.670	1.00 17.46	D

ATOM	3252	CG	TYR	D	34	94.508	41.970	26.588	1.00 20.90	D
MOTA	3253	CD1	TYR	D	34	95.488	41.390	27.391	1.00 21.91	D
ATOM	3254	CE1	TYR		34	96.295	42.174	28.221	1.00 24.17 1.00 20.26	D D
ATOM	3255	CD2 CE2	TYR TYR		34 34	94.351 95.147	43.354 44.141	26.638 27.463	1.00 20.26 1.00 24.97	D
ATOM ATOM	3256 3257	CEZ	TYR		34	96.117	43.546	28.251	1.00 23.87	D
ATOM	3258	OH	TYR		34	96.904	44.326	29.065	1.00 26.29	D
ATOM	3259	C	TYR		34	92.766	39.836	27.642	1.00 16.56	D
ATOM	3260	0	TYR	D	34	92.476	40.386	28.699	1.00 15.36	D
MOTA	3261	N	VAL		35	93.354	38.653	27.586	1.00 18.29	D
ATOM	3262	CA	VAL		35	93.768	37.971	28.795	1.00 19.11	D D
ATOM	3263	CB	VAL VAL		35 35	93.257 93.910	36.514 35.780	28.842 29.992	1.00 17.61 1.00 17.99	D
ATOM ATOM	3264 3265	CG1 CG2	VAL		35	91.744	36.493	29.003	1.00 17.82	D
ATOM	3266	C	VAL		35	95.290	37.950	28.813	1.00 19.96	D
ATOM	3267	0	VAL		35	95.914	37.492	27.866	1.00 17.73	D
MOTA	3268	N	ASP	D	36	95.883	38.473	29.880	1.00 22.63	D
ATOM	3269	CA	ASP		36	97.333	38.456	30.005	1.00 24.79	D
ATOM	3270	CB	ASP		36 36	97.795 99.298	39.409 39.574	31.106 31.131	1.00 26.41 1.00 30.12	, D
ATOM ATOM	3271 3272	CG OD1	ASP ASP	D D	,36 36	100.002	38.547	31.252	1.00 32.04	D
ATOM	3272	OD2		D	36	99.776	40.726	31.028	1.00 32.20	D
ATOM	3274	C		D	36	97.650	37.011	30.389	1.00 25.23	D
MOTA	3275	0	ASP	D	36	97.349	36.575	31.502	1.00 25.21	D
ATOM	3276	N	LEU		37	98.236	36.272	29.455	1.00 23.64	D
ATOM	3277	CA	LEU		37	98.549	34.870 34.232	29.676 28.355	1.00 25.25 1.00 21.08	D D
ATOM	3278 3279	CB CG	LEU		37 37	98.992 97.955	34.252	27.225	1.00 20.24	Đ
ATOM ATOM	3279	CD1			37	98.568	33.934	25.899	1.00 17.23	D
ATOM	3281	CD2			37	96.730	33.516	27.541	1.00 19.11	D
MOTA	3282	C	LEU	D	37	99.590	34.626	30.770	1.00 27.73	D
ATOM	3283	0	LEU		37	99.464	33.682	31.554	1.00 27.92	D
ATOM	3284	N	GLY		38	100.608	35.474 35.292	30.837 31.851	1.00 29.31 1.00 30.44	D D
ATOM	3285 3286	CA C	GLY		38 38	101.629 101.141	35.232	33.242	1.00 30.44	D
ATOM ATOM	3280	0	GLY		38	101.502	34.986	34.220	1.00 34.37	D
ATOM	3288	N	ARG		39	100.309	36.669	33.335	1.00 35.10	D
ATOM	3289	CA	ARG	D	39	99.786	37.103	34.623	1.00 36.92	D
ATOM	3290	CB	ARG		39	99.693	38.632	34.653	1.00 39.96	D
ATOM	3291	CG	ARG		39	101.011	39.318	34.301	1.00 44.57 1.00 49.71	D D
ATOM	3292	CD	ARG ARG		39 39	101.006 102.240	40.798 41.484	34.667 34.270	1.00 53.08	D
ATOM ATOM	3293 3294	NE CZ	ARG		39	103.460	41.164	34.698	1.00 55.33	D
ATOM	3295	NH1			39	103.635	40.158	35.546	1.00 56.98	D
MOTA	3296	NH2	ARG	D	39	104.512	41.859	34.282	1.00 56.80	D
MOTA	3297	C	ARG		39	98.429	36.476	34.924	1.00 35.86	D
MOTA	3298	0	ARG		39	97.886	36.630 35.757	36.022 33.944	1.00 35.27 1.00 34.51	D D
ATOM	3299 3300	N CA	LYS LYS		40 40	97.893 96.602	35.757	34.090	1.00 33.49	D
ATOM ATOM	3300	CB	LYS		40	96.714	33.939	35.088	1.00 34.77	D
ATOM	3302	CG	LYS		40	95.482	33.040	35.133	1.00 41.38	D
MOTA	3303	CD	LYS	D	40	95.703	31.839	36.046	1.00 45.02	D
MOTA	3304	CE	LYS		40	94.443	31.001	36.185 37.112	1.00 46.54 1.00 48.98	D D
ATOM	3305	NZ	LYS LYS		40 40	94.652 95.511	29.853 36.064	34.542	1.00 \(\frac{1}{3} \).95	D
ATOM ATOM	3306 3307	C O	LYS			94.780	35.794	35.492	1.00 28.23	D
ATOM	3308	N	GLU			95.401	37.197	33.858	1.00 30.54	D
MOTA	3309	CA	GLU	D	41	94.384	38.175	34.210	1.00 30.41	D
ATOM	3310	CB	GLU			94.980	39.302	35.078	1.00 34.10	D
ATOM	3311	CG	GLU			96.180 96.834	40.034	34.488 35.482	1.00 41.52 1.00 45.72	D D
ATOM ATOM	3312 3313	CD OE 3	GLU GLU			97.826	41.665	35.108	1.00 48.68	D
ATOM	3314	OE2				96.362	41.086	36.638	1.00 47.60	D
ATOM	3315	C	GLU			93.651	38.766	33.014	1.00 28.03	D
MOTA	3316	0	GLU	J D	41	94.220	38.981	31.940	1.00 25.49	D
MOTA	3317	N	THE			92.364		33.226	1.00 25.48	D
ATOM	3318	CA	THR			91.488 90.035	39.582	32.224 32.511	1.00 23.42 1.00 22.07	D D
MOTA MOTA	3319 3320	CB OG:	THR L THR			89.927	39.187 37.761	32.511	1.00 22.07	D
ATOM	3320	CG2				89.087	39.817	31.497	1.00 20.32	D
ATOM	3322	C	THE			91.615	41.098	32.301	1.00 22.29	D
ATOM	3323	0	THE		42	91.492	41.680	33.373	1.00 21.54	D
MOTA	3324	N	VAI		_	91.874		31.167	1.00 21.50	D D
ATOM	3325	CA	VAI	, D	43	92.004	43.183	31.136	1.00 19.88	ע
								20		

ATOM 3326 CE VAL D 43 93.428 43.584 30.697 1.00 21.56 ATOM 3327 CG1 VAL D 43 93.620 45.091 30.828 1.00 20.99 ATOM 3328 CG2 VAL D 43 94.456 42.827 31.539 1.00 19.79 ATOM 3328 C VAL D 43 94.456 42.827 31.539 1.00 19.79 ATOM 3330 O VAL D 43 91.045 43.513 28.959 1.00 19.79 ATOM 3331 N FEP D 44 89.987 44.466 30.690 1.00 21.49 ATOM 3332 CA TRP D 44 88.946 45.028 29.836 1.00 22.48 ATOM 3332 CB TRP D 44 87.685 45.326 30.649 1.00 21.57 ATOM 3335 CD2 TRP D 44 87.685 45.326 30.649 1.00 21.57 ATOM 3336 CE2 TRP D 44 86.280 43.125 30.854 1.00 22.20 ATOM 3337 CE3 TRP D 44 86.280 43.125 30.854 1.00 22.20 ATOM 3336 CD2 TRP D 44 86.119 42.150 31.862 1.00 22.20 ATOM 3337 CE3 TRP D 44 87.492 43.736 32.633 1.00 23.17 ATOM 3338 NEI TRP D 44 86.886 42.548 29.836 1.00 22.19 ATOM 3340 CZ2 TRP D 44 86.886 42.548 32.937 1.00 23.17 ATOM 3341 CZ3 TRP D 44 86.886 42.548 32.937 1.00 23.17 ATOM 3341 CZ2 TRP D 44 86.886 42.548 32.937 1.00 23.17 ATOM 3341 CZ2 TRP D 44 86.886 42.548 32.937 1.00 24.30 ATOM 3342 CH2 TRP D 44 86.886 42.548 32.937 1.00 24.30 ATOM 3343 C TRP D 44 86.866 40.870 30.487 1.00 24.30 ATOM 3343 C TRP D 44 84.807 41.824 99.461 1.00 24.30 ATOM 3343 C TRP D 44 84.807 41.824 99.461 1.00 24.30 ATOM 3343 C TRP D 44 89.425 46.291 29.143 1.00 24.05 ATOM 3345 N CWS D 45 89.998 46.417 27.859 1.00 24.24 ATOM 3346 CA CWS D 45 89.998 46.417 27.859 1.00 24.24 ATOM 3345 C C WS D 45 89.998 46.417 27.859 1.00 24.24 ATOM 3345 C C WS D 45 89.998 46.417 27.859 1.00 24.24 ATOM 3345 C C CWS D 45 89.998 46.417 27.859 1.00 24.24 ATOM 3355 C C LBU D 46 86.002 49.087 27.232 1.00 27.07 ATOM 3356 C C WS D 45 89.991 47.141 25.672 1.00 25.96 ATOM 3357 C LBU D 46 86.002 49.087 27.232 1.00 27.07 ATOM 3356 C C WS D 45 88.377 48.608 26.995 1.00 27.07 ATOM 3356 C C WS D 46 86.902 49.987 27.232 1.00 28.23 ATOM 3356 C C WS D 46 86.902 49.987 27.232 1.00 28.23 ATOM 3356 C C WS D 46 86.902 49.987 27.232 1.00 28.23 ATOM 3356 C C WS D 46 86.902 49.987 27.232 1.00 28.23 ATOM 3356 C C WS D 46 86	
ATOM 3328 CG2 VAL D 43 99.4.456 42.827 31.539 1.00 19.79 ATOM 3329 C VAL D 43 90.968 43.744 30.164 1.00 20.50 ATOM 3330 O VAL D 43 91.045 43.513 28.559 1.00 19.49 ATOM 3331 N TRP D 44 89.987 44.466 30.650 1.00 21.49 ATOM 3331 N TRP D 44 88.946 45.022 29.836 1.00 22.88 ATOM 3333 CB TRP D 44 87.685 45.326 30.649 1.00 21.57 ATOM 3333 CB TRP D 44 87.685 45.326 30.649 1.00 22.88 ATOM 3335 CD2 TRP D 44 86.119 42.150 31.862 1.00 22.20 ATOM 3336 CE2 TRP D 44 86.119 42.150 31.862 1.00 22.20 ATOM 3337 CE3 TRP D 44 86.119 42.150 31.862 1.00 22.20 ATOM 3338 CD1 TRP D 44 85.611 42.951 29.634 1.00 20.96 ATOM 3339 NEI TRP D 44 85.611 42.951 29.634 1.00 20.96 ATOM 3339 NEI TRP D 44 86.868 42.848 32.937 1.00 23.17 ATOM 3339 NEI TRP D 44 86.868 42.848 32.937 1.00 23.70 ATOM 3340 CZ2 TRP D 44 86.868 42.848 32.937 1.00 23.70 ATOM 3341 CZ3 TRP D 44 86.868 42.848 32.937 1.00 23.70 ATOM 3341 CZ3 TRP D 44 86.866 40.870 30.467 1.00 24.30 ATOM 3341 CZ3 TRP D 44 84.807 41.824 29.461 1.00 22.81 ATOM 3342 CR2 TRP D 44 84.807 41.824 29.461 1.00 24.05 ATOM 3343 C TRP D 44 84.807 41.824 29.461 1.00 24.05 ATOM 3344 C TRP D 44 89.425 46.291 29.143 1.00 24.05 ATOM 3344 C TRP D 44 89.425 46.291 29.143 1.00 24.05 ATOM 3344 C TRP D 44 89.425 46.291 29.143 1.00 24.50 ATOM 3347 CB CYS D 45 89.98 47.800 27.069 1.00 26.23 ATOM 3347 CB CYS D 45 89.98 47.500 27.069 1.00 26.23 ATOM 3347 CB CYS D 45 89.98 47.500 27.069 1.00 26.23 ATOM 3348 SG CYS D 45 89.98 47.500 27.07 B.00 24.24 ATOM 3350 C CYS D 45 89.98 47.500 27.07 B.00 24.24 ATOM 3350 C CYS D 45 89.99 46.417 27.859 1.00 24.25 ATOM 3351 N LEU D 46 87.1757 48.99 27.222 1.00 25.96 ATOM 3354 CR LEU D 46 87.157 48.99 32.72.73 1.00 27.18 ATOM 3355 CD LEU D 46 84.907 48.508 25.951 1.00 29.70 ATOM 3355 C DL LEU D 46 84.907 48.508 25.951 1.00 29.97 ATOM 3356 CP LEU D 46 84.907 48.509 29.318 1.00 29.97 ATOM 3356 CP LEU D 46 85.504 49.133 29.216 1.00 29.97 ATOM 3356 CP LEU D 46 85.504 49.133 29.216 1.00 29.97 ATOM 3356 CP LEU D 46 85.504 49.133 29.216 1.00 29.97 ATOM 3356 CP LEU D 46 85.504 49.133 29.236 1.00 2	
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ATOM 3361 CA PRO D 47 85.182 50.533 30.709 1.00 29.01 ATOM 3362 CB PRO D 47 85.139 52.051 30.806 1.00 29.32 ATOM 3363 CG PRO D 47 86.307 52.447 29.929 1.00 30.61 ATOM 3364 C PRO D 47 83.879 49.875 31.169 1.00 28.51 ATOM 3365 O PRO D 47 83.867 49.151 32.163 1.00 28.22 ATOM 3366 N VAL D 48 82.784 50.126 30.458 1.00 28.05 ATOM 3367 CA VAL D 48 81.492 49.545 30.826 1.00 27.41 ATOM 3368 CB VAL D 48 80.406 49.918 29.810 1.00 26.31 ATOM 3370 CG2 VAL D 48 80.949 49.744 28.398 1.00 26.11 ATOM 3371 C VAL D 48 80.949 49.744 28.398 1.00 26.77 ATOM 3372 O VAL D 48 80.622 47.462 31.627 1.00 27.43 ATOM 3373 N LEU D 49 82.449 47.353 30.332 1.00 27.43 ATOM 3375 CB LEU D 49 82.517 45.898 30.395 1.00 27.47 ATOM 3376 CG LEU D 49 82.405 44.886 27.944 1.00 29.74 ATOM 3377 CD1 LEU D 49 81.361 45.898 27.578 1.00 29.28 ATOM 3377 CD1 LEU D 49 83.329 44.627 26.753 1.00 27.21 ATOM 3377 CD1 LEU D 49 83.329 44.627 26.753 1.00 27.47 ATOM 3377 CD1 LEU D 49 83.329 44.627 26.753 1.00 27.27 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 27.47 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 27.72 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 27.72 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 27.72 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 27.72	D
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ATOM 3365 O PRO D 47 ATOM 3366 N VAL D 48 ATOM 3366 N VAL D 48 ATOM 3367 CA VAL D 48 ATOM 3368 CB VAL D 48 ATOM 3369 CG1 VAL D 48 ATOM 3370 CG2 VAL D 48 ATOM 3371 C VAL D 48 ATOM 3372 O VAL D 48 ATOM 3373 N LEU D 49 ATOM 3374 CA LEU D 49 ATOM 3375 CB LEU D 49 ATOM 3376 CG LEU D 49 ATOM 3377 CD1 LEU D 49 ATOM 3377 CD1 LEU D 49 ATOM 3377 CD1 LEU D 49 ATOM 3378 CD2 LEU D 49 ATOM 3388 CD2 LEU D 49 ATOM 3388 CD2 LEU D 49 ATOM 3388 CD2 LEU D 49	D
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ATOM 3367 CA VAL D 48 81.492 49.545 30.826 1.00 27.41 ATOM 3368 CB VAL D 48 80.406 49.918 29.810 1.00 26.31 ATOM 3369 CG1 VAL D 48 79.955 51.345 30.027 1.00 30.25 ATOM 3370 CG2 VAL D 48 80.949 49.744 28.398 1.00 26.11 ATOM 3371 C VAL D 48 81.490 48.022 30.961 1.00 26.77 ATOM 3372 O VAL D 48 80.622 47.462 31.627 1.00 27.43 ATOM 3373 N LEU D 49 82.449 47.353 30.332 1.00 25.75 ATOM 3374 CA LEU D 49 82.517 45.898 30.395 1.00 27.21 ATOM 3375 CB LEU D 49 83.237 45.354 29.153 1.00 27.47 ATOM 3376 CG LEU D 49 82.405 44.886 27.944 1.00 29.74 ATOM 3377 CD1 LEU D 49 81.361 45.898 27.578 1.00 29.28 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 29.72	D
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ATOM 3373 N LEU D 49 82.449 47.353 30.332 1.00 25.75 ATOM 3374 CA LEU D 49 82.517 45.898 30.395 1.00 27.21 ATOM 3375 CB LEU D 49 83.237 45.354 29.153 1.00 27.47 ATOM 3376 CG LEU D 49 82.405 44.886 27.944 1.00 29.74 ATOM 3377 CD1 LEU D 49 81.361 45.898 27.578 1.00 29.28 ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 29.72	D
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ATOM 3378 CD2 LEU D 49 83.329 44.627 26.753 1.00 29.72	D
20 10 17 27 27 17 27 27 27 27 27 27 27 27 27 27 27 27 27	D
	D
ATOM 3380 O LEU D 49 83.246 44.163 31.900 1.00 25.45	D -
ATOM 3381 N ARG D 50 83.680 46.283 32.508 1.00 29.82	D
ATOM 3382 CA ARG D 50 84.319 45.892 33.768 1.00 32.18	D D
ATOM 3383 CB ARG D 50 84.900 47.105 34.509 1.00 35.49 ATOM 3384 CG ARG D 50 86.010 47.890 33.824 1.00 40.53	D
A10M 3304 CG 14CC 2	D
ATOM 3385 CD ARG D 50 86.524 48.968 34.786 1.00 42.89 ATOM 3386 NE ARG D 50 87.297 50.017 34.125 1.00 46.26	D
ATOM 3387 CZ ARG D 50 88.484 49.836 33.555 1.00 46.43	D
ATOM 3388 NH1 ARG D 50 89.049 48.636 33.564 1.00 46.42	D
ATOM 3389 NH2 ARG D 50 89.100 50.857 32.968 1.00 43.78	D
ATOM 3390 C ARG D 50 83.283 45.247 34.690 1.00 31.58	D
ATOM 3391 O ARG D 50 83.631 44.577 35.664 1.00 31.56	D D
AIOM 3592 N GIIN B 32 02.000 20.000 35 001 1 00 20 10	D
ATOM 3393 CA GLN D 51 80.942 44.921 35.221 1.00 30.10 ATOM 3394 CB GLN D 51 79.610 45.592 34.880 1.00 31.37	ם
MIOM 3394 CB 3227 2 22 707 45 45 450 22 406 1 00 22 44	D
ATOM 3395 CG GLN D 51 79.194 45.469 33.426 1.00 33.44 ATOM 3396 CD GLN D 51 77.888 46.188 33.144 1.00 37.07	
ATOM 3396 CD GLN D 51 77.000 10.200 2	D
ATOM 3398 NE2 GLN D 51 77.951 47.222 32.309 1.00 34.55	
ATOM 3399 C GLN D 51 80.830 43.411 35.049 1.00 29.51	D

MOTA	3400	0	GLN	D	51	80.291	42.721	35.911	1.00 29.09	D
MOTA	3401	N		D	52	81.342	42.899	33.935	1.00 28.19	D
ATOM	3402	CA		D D	52 52	81.300 81.218	41.468 41.188	33.676 32.178	1.00 26.27 1.00 25.00	D D
ATOM ATOM	3403 3404	CB CG		D	52 52	80.030	41.801	31.513	1.00 23.07	D
ATOM	3405	CD1		D	52	78.744	41.569	31.999	1.00 22.75	D
MOTA	3406	CD2		D	52	80.188	42.594	30.380	1.00 23.46	D
MOTA	3407	CE1	PHE	D	52	77.627	42.122	31.364	1.00 21.26	D
ATOM	3408	CE2	PHE	D	52	79.079	43.151	29.735	1.00 21.92	D
ATOM	3409	CZ		D	52	77.799	42.913	30.231	1.00 21.69	D
ATOM	3410	C		D	52 52	82.547 83.477	40.797 41.461	34.217 34.669	1.00 27.11 1.00 27.64	D D
ATOM ATOM	3411 3412	N O	PHE		52 53	82.556	39.471	34.152	1.00 27.25	D
MOTA	3413	CA	ARG		53	83.683	38.672	34.609	1.00 28.31	Ð
ATOM	3414	CB	ARG		53	83.347	37.976	35.939	1.00 32.75	D
MOTA	3415	CG	ARG	D	53	83.263	38.921	37.143	1.00 40.59	D
MOTA	3416	CD	ARG	D	53	82.418	38.325	38.269	1.00 45.99	D
MOTA	3417	NE	ARG		53	81.007	38.229	37.892	1.00 52.14	D
ATOM	3418	CZ	ARG		53	80.172	39.265 40.493	37.808 38.080	1.00 53.70 1.00 53.85	D D
MOTA	3419 3420	NH1 NH2	ARG ARG		53 53	80.597 78.910	39.071	37.440	1.00 54.61	D
ATOM ATOM	3421	C	ARG		53	84.007	37.624	33.548	1.00 25.73	D
ATOM	3422	0	ARG		53	83.120	37.103	32.875	1.00 23.84	D
MOTA	3423	N	PHE	D	54	85.290	37.335	33.387	1.00 23.47	D
ATOM	3424	CA	PHE	D	54	85.716	36.336	32.425	1.00 19.92	D
ATOM	3425	CB		D	54	86.159	36.980	31.113	1.00 15.46	D
MOTA	3426	CG	PHE		5 4	86.346	35.994	30.007	1.00 17.29 1.00 15.32	D D
ATOM	3427	CD1	PHE	D	54 54	85.249 87.615	35.506 35.503	29.303 29.701	1.00 15.32	D
ATOM ATOM	3428 3429	CD2 CE1	PHE		54 54	85.415	34.539	28.309	1.00 16.04	D
ATOM	3430	CE2	PHE		54	87.788	34.535	28.709	1.00 13.99	D
ATOM	3431	CZ	PHE		54	86.688	34.055	28.014	1.00 14.35	D
MOTA	3432	C	PHE	D	54	86.879	35.598	33.055	1.00 18.63	D
MOTA	3433	O	PHE		54	87.922	36.188	33.329	1.00 19.50	D
MOTA	3434	N	ASP		55	86.676	34.312	33.309	1.00 19.05 1.00 19.33	D D
ATOM	3435	CA	ASP		55 55	87.689 87.084	33.466 32.100	33.921 34.237	1.00 19.33 1.00 21.38	D
ATOM ATOM	3436 3437	CB CG	ASP ASP		55 55	88.090	31.138	34.832	1.00 24.95	D
ATOM	3438	OD1	ASP		55 55	89.264	31.528	35.021	1.00 27.01	D
ATOM	3439	OD2			55	87.703	29.985	35.112	1.00 27.48	D
ATOM	3440	C	ASP	D	55	88.863	33.323	32.955	1.00 19.84	D
MOTA	3441	0	ASP	D	55	88.741	32.691	31.904	1.00 18.07	D
ATOM	3442	N	PRO		56	90.024	33.909	33.311 34.593	1.00 19.36 1.00 16.09	D D
ATOM	3443	CD	PRO PRO		56 56	90.285 91.240	34.584 33.867	34.593	1.00 18.34	D
ATOM ATOM	3444 3445	CA CB	PRO		56	92.228	34.729	33.278	1.00 19.78	D
ATOM	3446	CG	PRO		56	91.792	34.517	34.692	1.00 18.66	D
ATOM	3447	C	PRO		56	91.770	32.468	32.206	1.00 18.30	D
MOTA	3448	0	PRO	D	56	92.583	32.277	31.299	1.00 17.41	D
MOTA	3449	N	GLN		57	91.304	31.489	32.977	1.00 18.31	D
MOTA	3450	CA	GLN		57 57	91.744	30.114	32.781	1.00 18.39 1.00 19.94	D D
MOTA	3451	CB	GLN GLN		57 57	91.314 91.738	29.233 27.773	33.963 33.856	1.00 19.54	D
ATOM ATOM	3452 3453	CG CD	GLN		5 <i>7</i>	93.252	27.73	33.765	1.00 23.86	D
MOTA	3454	OE1			5 <i>7</i>	94.000		34.612	1.00 23.68	D
ATOM	3455	NE2			57	93.709	26.885	32.739	1.00 19.56	D
MOTA	3456	C	GLN	D	57	91.174		31.480	1.00 20.01	D
ATOM	3457	0	GLN		57	91.733		30.903	1.00 19.26	D
ATOM	3458	N	PHE		58	90.059		31.016	1.00 19.19 1.00 20.37	D D
ATOM	3459	CA	PHE		58 58	89.490 88.178		29.765 29.427	1.00 20.57	D
MOTA MOTA	3460 3461	CB CG	PHE		58	87.587			1.00 20.67	D
ATOM	3462	CD1			58	88.040			1.00 19.84	D
ATOM	3463	CD2			58	86.640	28.891	28.070	1.00 19.87	D
ATOM	3464	CE1		D	58	87.562		25.682	1.00 19.25	D
ATOM	3465	CE2			58	86.156			1.00 20.67	D
MOTA	3466	CZ	PHE		58	86.623			1.00 19.50 1.00 20.46	D D
MOTA	3467	C	PHE			90.508 90.745			1.00 20.46	D D
MOTA	3468 3469	N O	ALA			91.115			1.00 20.85	D
ATOM ATOM	3469	CA	ALA			92.111	•		1.00 21.87	D
MOTA	3471	CB	ALA			92.458				D
ATOM	3472	C	ALA			93.374			1.00 22.41	D
ATOM	3473	0	ALA	D	59	93.877	30.151	26.796	1.00 22.54	D

ATOM	3474	N	LEU	D	60	93.890	30.409	29.030	1.00 21.24	D
ATOM	3475	CA	LEU		60	95.101	29.601	29.188	1.00 22.31	D
ATOM	3476	CB	LEU	D	60	95.501	29.474	30.663	1.00 22.79	D
ATOM	3477	CG	LEU	D	60	96.063	30.698	31.393	1.00 25.87	D
ATOM	3478	CD1	LEU	D	60	96.455	30.303	32.805	1.00 28.75	D
ATOM	3479	CD2		D	60	97.270	31.223	30.670	1.00 28.42	D
MOTA	3480	C		D	60	94.891	28.207	28.617	1.00 21.85	D
ATOM	3481	0		D	60	95.731	27.691	27.875	1.00 22.48 1.00 19.32	D D
ATOM	3482	N		D	61	93.763	27.600 26.259	28.966 28.489	1.00 19.32	D
ATOM	3483	CA		D	61 61	93.457 92.175	25.721	29.158	1.00 20.04	D
ATOM	3484	CB OG1		D D	61	92.175	25.721	30.558	1.00 23.09	D
ATOM ATOM	3485 3486	CG2		D	61	91.759	24.393	28.546	1.00 21.15	D
ATOM	3487	C	THR		61	93.283	26.240	26.974	1.00 19.50	D
ATOM	3488	0	THR		61	93.805	25.363	26.288	1.00 18.76	D
ATOM	3489	N	ASN		62	92.565	27.229	26.456	1.00 19.66	D
ATOM	3490	CA	ASN	D	62	92.310	27.300	25.032	1.00 19.00	D
ATOM	3491	CB	ASN	D	62	91.356	28.453	24.729	1.00 18.52	D
ATOM	3492	CG	ASN	D	62	90.262	28.052	23.760	1.00, 20.31	D
ATOM	3493	OD1	ASN	D	62	89.726	26.942	23.833	1.00 19.27	D
ATOM	3494	ND2	ASN	D	62	89.917	28.952	22.854	1.00 22.25	D
ATOM	3495	C	ASN		62	93.599	27.445	24.244	1.00 19.63	D
ATOM	3496	0	ASN		62	93.774	26.788	23.221	1.00 21.16	D D
ATOM	3497	N	ILE	D	63	94.509	28.290	24.724	1.00 19.68	D
ATOM	3498	CA	ILE		63	95.779	28.481	24.033 24.645	1.00 18.76 1.00 18.72	D
ATOM	3499	CB	ILE		63	96.587 97.946	29.660 29.780	23.966	1.00 13.72	D
ATOM	3500	CG2			63 63	97.946	30.968	24.471	1.00 17.09	D
ATOM	3501	CG1 CD1	ILE ILE		63	95.507	31.313	23.017	1.00 17.47	D
ATOM	3502 3503	CDI	ILE		63	96.613	27.195	24.094	1.00 18.86	D
ATOM ATOM	3503	0	ILE		63	97.354	26.885	23.164	1.00 20.67	D
ATOM	3505	N	ALA		64	96.497	26.448	25.188	1.00 18.22	D
ATOM	3506	CA	ALA		64	97.244	25.193	25.316	1.00 20.33	D
ATOM	3507	CB	ALA		64	97.039	24.574	26.708	1.00 17.30	D
ATOM	3508	C	ALA	D	64	96.756	24.232	24.233	1.00 21.38	D
ATOM	3509	0	ALA	D	64	97.536	23.459	23.677	1.00 23.44	D
MOTA	3510	N	VAL	D	65	95.459	24.290	23.940	1.00 21.97	D
MOTA	3511	CA	VAL	D	65	94.872	23.444	22.910	1.00 22.59	D
ATOM	3512	CB	VAL	D	65	93.324	23.570	22.890	1.00 22.30	D
ATOM	3513	CG1			65	92.744	22.781	21.728	1.00 17.73	D
MOTA	3514	CG2			65	92.747	23.053	24.204	1.00 19.10	D
ATOM	3515	C	VAL		65	95.441	23.832	21.541	1.00 23.65 1.00 23.24	D D
ATOM	3516	0	VAL		65 66	95.783	22.961 25.133	20.746 21.271	1.00 25.24	D
ATOM	3517	N	LEU		66 66	95.552 96.102	25.580	19.991	1.00 25.05	D
MOTA	3518	CA CB	LEU LEU		66	96.104	27.111	19.870	1.00 23.98	Ď
ATOM ATOM	3519 3520	CG	LEU		66	94.826	27.953	19.969	1.00 25.20	D
ATOM	3521	CD1			66	95.030	29.233	19.169	1.00 21.70	D
ATOM	3522	CD2			66	93.629	27.211	19.435	1.00 26.16	D
ATOM	3523	C	LEU	D	66	97.533	25.078	19.880	1.00 26.24	D
ATOM	3524	0	LEU	D	66	97.971	24.667	18.816	1.00 27.10	D
ATOM	3525	N	LYS	D	67	98.262	25.131	20.989	1.00 27.93	Ð
MOTA	3526	CA	LYS		67	99.642	24.658	21.024	1.00 28.00	D
ATOM	3527	CB	LYS		67	100.215	24.827	22.437	1.00 27.69	D
ATOM	3528	CG	LYS		67	101.633	24.316	22.625	1.00 28.46	D D
ATOM	3529	CD	LYS		67 67	102.086	24.504	24.069 24.356	1.00 30.94 1.00 32.95	D
MOTA	3530	CE	LYS		67 67	103.401 104.517	23.791 24.279	23.503	1.00 35.64	D
ATOM	3531	NZ	LYS LYS		67 67	99.642	23.182	20.629	1.00 27.56	D
MOTA	3532 3533	C O	LYS		67	100.414	22.759	19.767	1.00 27.65	D
MOTA MOTA	3534	И	HIS		68	98.761	22.405	21.254	1.00 27.05	D
ATOM	3535	CA	HIS		68	98.665	20.982	20.956	1.00 26.31	D
MOTA	3536	CB	HIS		68	97.600		21.844	1.00 27.74	D
ATOM	3537	CG	HIS		68	97.356		21.531	1.00 31.20	D
ATOM	3538	CD2	2 HIS	D	68	97.801	17.748	22.130	1.00 31.26	D
ATOM	3539	ND	L HIS	D	68	96.582	18.466	20.465	1.00 32.71	D
ATOM	3540	CE:	L HIS	D	68	96.560		20.423	1.00 31.32	D
MOTA	3541	NE:	2 HIS	S D	68	97.292			1.00 31.58	D
MOTA	3542	C	HIS		68	98.341			1.00 25.27	D
MOTA	3543	0	HIS		68	98.958			1.00 25.67	D
MOTA	3544	N	ASI		69	97.386	_		1.00 22.00	D
ATOM	3545	CA	ASI		69 60	96.986	_		1.00 23.20 1.00 23.27	D D
ATOM	3546	CB	ASI		69	95.706	_		1.00 23.27	D
ATOM	3547	CG	ASI	1 D	69	94.447	21.504	£7.00D	L.UU AT.AU	ט

ATOM	3548	COL	ASN	D	69	94.521	20.536	18.562	1.00 26.69	D
ATOM	3549	ND2	ASN		69	93.283	21.994	17.381	1.00 21.03	D
ATOM	3550	C	ASN	D	69	98.091	21.855	16.601	1.00 24.52	D
ATOM	3551	0	ASN	D	69	98.329	21.223	15.570	1.00 22.82	D
ATOM	3552	N	LEU	D	70	98.763	22.954	16.934	1.00 24.56	D
ATOM	3553	CA	LEU	D	70	99.831	23.459	16.078	1.00 26.89	D
ATOM	3554	CB	LEU	D	70	100.478	24.707	16.690	1.00 23.85	D
ATOM	3555	CG	LEU	D	70	101.619	25.306	15.857	1.00 22.71	D
ATOM	3556	CD1	LEU	D	70	101.082	25.776	14.519	1.00 19.18	D
ATOM	3557	CD2	LEU	D	70	102.254	26.472	16.592	1.00 23.62	D
ATOM	3558	C	LEU	D	70	100.900	22.388	15.882	1.00 28.63	D
ATOM	3559	0	LEU	D	70	101.413	22.210	14.780	1.00 27.56	D
ATOM	3560	N	ASN	D	71	101.224	21.687	16.967	1.00 31.13	D
ATOM	3561	CA	ASN	D	71	102.238	20.637	16.962	1.00 35.25	D
ATOM	3562	CB	ASN	D	71	102.393	20.052	18.370	1.00 35.30	D
ATOM	3563	CG	ASN	D	71	103.149	20.978	19.307	1.00 38.03	D
MOTA	3564	OD1	ASN	D	71	103.197	20.751	20.518	1.00 40.05	D
ATOM	3565	ND2	ASN	D	71	103.752	22.026	18.748	1.00 38.78	D
ATOM	3566	C	ASN	D	71	101.931	19.521	15.975	1.00 36.85	D
ATOM	3567	0	ASN	D	71	102.829	18.997	15.316	1.00 36.91	D
ATOM	3568	N	SER	D	72	100.660	19.157	15.876	1.00 38.08	D
ATOM	3569	CA	SER	D	72	100.261	18.104	14.961	1.00 39.44	D
MOTA	3570	CB	SER	D	72	98.847	17.623	15.306	1.00 40.69	D
ATOM	3571	OG	SER	D	72	98.529	16.427	14.611	1.00 44.84	D
ATOM	3572	C	SER	D	72	100.320	18.614	13.520	1.00 39.55	D
MOTA	3573	0	SER	D	72	100.798	17.915	12.625	1.00 38.61	D
ATOM	3574	N	LEU	D	73	99.846	19.839	13.305	1.00 40.64	D
MOTA	3575	$\mathbf{C}\mathbf{A}$	LEU	D	73	99.844	20.443	11.974	1.00 42.19	D
ATOM	3576	СВ	LEU	D	73	99.085	21.768	11.990	1.00 42.17	D
ATOM	3577	CG	LEU	D	73	97.608	21.700	11.608	1.00 43.12	D
MOTA	3578	CD1	LEU	D	73	96.891	20.664	12.443	1.00 44.19	D
ATOM	3579	CD2	LEU	D	73	96.988	23.072	11.801	1.00 44.59	D
MOTA	3580	C	LEU	D	73	101.237	20.678	11.407	1.00 43.27	D
ATOM	3581	0	LEU	D	73	101.466	20.479	10.215	1.00 43.00	D
ATOM	3582	N	ILE	D	74	102.162	21.116	12.253	1.00 44.60	D
ATOM	3583	CA	ILE	D	74	103.529	21.364	11.812	1.00 46.44	D
ATOM	3584	CB	ILE	D	74	104.431	21.770	13.000	1.00 46.31	D
MOTA	3585	CG2	ILE	D	74	105.893	21.792	12.571	1.00 46.14	D
ATOM	3586	CG1	ILE	D	74	103.996	23.140	13.529	1.00 45.97	D
ATOM	3587	CD1	ILE	D	74	104.683	23.561	14.812	1.00 43.97	D
ATOM	3588	C	ILE	D	74	104.077	20.095	11.166	1.00 48.14	D
MOTA	3589	0	ILE	D	74	104.724	20.147	10.119	1.00 48.28	D
ATOM	3590	N	LYS	D	75	103.800	18.957	11.795	1.00 49.68	D -
ATOM	3591	CA	LYS	D	75	104.252	17.669	11.290	1.00 51.82	D
MOTA	3592	CB	LYS	D	75	104.060	16.589	12.356	1.00 52.85	D
ATOM	3593	CG	LYS	D	75	104.856	16.839	13.621	1.00 54.78	D
MOTA	3594	CD	LYS	D	75	104.517	15.831	14.704	1.00 57.28	D
MOTA	3595	CE	LYS	D	75	105.222	16.170	16.010	1.00 58.75	D
MOTA	3596	NZ	LYS		75	104.803	15.266	17.116	1.00 59.97	D
MOTA	3597	C	LYS		75	103.499	17.276	10.023	1.00 52.37	D
MOTA	3598	0	LYS			104.106	17.086	8.972	1.00 52.78	D
MOTA	3599	N	ARG		76	102.177	17.171	10.124	1.00 52.67	D
ATOM	3600	CA	ARG		76	101.353	16.783	8.986	1.00 52.67	D D
ATOM	3601	CB	ARG		76	99.911	16.546	9.439	1.00 53.54 1.00 55.62	D
MOTA	3602	CG	ARG		76	99.764	15.339	10.346 10.639	1.00 58.29	D
MOTA	3603	CD	ARG		76	98.310	15.011	11.319	1.00 58.25	D
ATOM	3604	NE	ARG		76	97.628	16.107 16.000	11.900	1.00 62.21	D
MOTA	3605	CZ	ARG			96.437	14.840	11.885	1.00 62.71	D
MOTA	3606	NH1				95.793	17.055	12.492	1.00 61.94	D
ATOM	3607	NH2				95.889	17.761	7.816	1.00 52.35	D
MOTA	3608	C	ARG			101.375	17.751	6.817	1.00 52.65	D
MOTA	3609	0	ARG			100.691	18.824	7.932	1.00 52.03	D
MOTA	3610	N	SER			102.160	19.807	6.856	1.00 51.87	D
ATOM	3611	CA	SER			102.255		7.379	1.00 50.95	D
ATOM	3612	CB	SER			101.945	21.212 21.668		1.00 30.93	D
ATOM	3613	OG	SER			102.975		6.233	1.00 48.11	D
ATOM	3614	C	SER			103.667	19.789		1.00 52.25	D
MOTA	3615	0	SER			104.028	20.633	6.731	1.00 51.87	D
ATOM	3616	N	ASN			104.455	18.814		1.00 52.79	D
MOTA	3617	CA	ASN			105.841	18.675		1.00 55.53	D
ATOM	3618	CB	ASN			105.912	18.364 17.901		1.00 55.33	D
MOTA	3619	CG	ASN			107.298	17.301		1.00 57.31	D
ATOM	3620	OD:				107.959	18.360	_	1.00 58.41	D
MOTA	3621	נתמ	2 ASN	נו ו	78	107.732	TO.200	5,104	50.05	****

ATOM	3622	С	ASN	מ	78	106.549	19.985	6.632	1.00 52.90	D
		_				107.300	20.536	5.826	1.00 53.98	D
ATOM	3623	0	ASN		78		·			
ATOM	3624	N	SER	D	79	106.275	20.479	7.835	1.00 51.25	D.
MOTA	3625	CA	SER	Ð	79	106.856	21.715	8.341	1.00 49.59	D
ATOM	3626	CB	SER	D	79	108.333	21.498	8.664	1.00 49.69	D
ATOM	3627	OG	SER	D	79	108.472	20.604	9.753	1.00 52.23	D
ATOM	3628	C	SER	Ð	79	106.711	22.931	7.437	1.00 47.21	D
		0	SER		79	107.699	23.588	7.111	1.00 47.49	D
ATOM	3629	_								D
ATOM	3630	N	THR		80	105.483	23.235	7.032	1.00 44.68	
MOTA	3631	CA	THR	D	80	105.245	24.401	6.189	1.00 43.69	D
MOTA	3632	CB	THR	D	80	103.928	24.274	5.407	1.00 45.12	D
ATOM	3633	OG1	THR	D	80	103.976	23.112	4.570	1.00 47.94	D
ATOM	3634	CG2	THR	D	80	103.706	25.505	4.541	1.00 44.11	D
ATOM	3635	C	THR		80	105.166	25.634	7.094	1.00 42.94	D
							25.783	7.874	1.00 41.60	D
ATOM	3636	0	THR		80	104.225				
ATOM	3637	N	ALA		81	106.162	26.510	6.988	1.00 40.39	D
MOTA	3638	CA	ALA	D	81	106.215	27.715	7.804	1.00 37.86	D
MOTA	3639	CB	ALA	D	81	107.657	28.171	7.958	1.00 39.23	D
ATOM	3640	С	ALA	D	81	105.372	28.846	7.234	1.00 36.29	D
ATOM	3641	0	ALA		81	104.988	28.829	6.065	1.00 35.21	D
		N	ALA		82	105.087	29.829	8.079	1.00 34.40	D
ATOM	3642							7.685	1.00 32.51	D
MOTA	3643	CA	ALA		82	104.294	30.984			
MOTA	3644	CB	ALA	Đ	82	103.915	31.789	8.920	1.00 32.45	D
ATOM	3645	C	ALA	D	82	105.064	31.866	6.707	1.00 32.78	D
ATOM	3646	0	ALA	D	82	106.294	31.913	6.740	1.00 30.87	D
ATOM	3647	N	THR	D	83	104.333	32.561	5.839	1.00 32.79	D
ATOM	3648	CA.	THR		83	104.940	33.459	4.867	1.00 34.48	D
		CB	THR		83	104,195	33.429	3.521	1.00 35.64	D
ATOM	3649						32.094	3.006	1.00 38.88	D
ATOM	3650	OG1	THR		83	104.179				
MOTA	3651	CG2	THR	D	83	104.880	34.342	2.521	1.00 35.33	D
MOTA	3652	C	THR	D	83	104.886	34.887	5.401	1.00 35.30	D
MOTA	3653	0	THR	D	83	103.827	35.355	5.824	1.00 36.88	D
MOTA	3654	N	ASN	D	84	106.025	35.575	5.379	1.00 35.07	D
ATOM	3655	CA	ASN		84	106.095	36.949	5.855	1.00 33.90	D
		CB	ASN		84	107.548	37.413	6.010	1.00 34.23	D
ATOM	3656							6.954	1.00 36.16	D
ATOM	3657	CG	ASN		84	108.351	36.545			
MOTA	3658	OD1	ASN	D	84	107.895	36.195	8.043	1.00 34.99	D
ATOM	3659	ND2	ASN	D	84	109.572	36.205	6.545	1.00 37.40	D
ATOM	3660	C	ASN	D	84	105.419	37.879	4.865	1.00 34.74	D
ATOM	3661	0	ASN	D	84	105.814	37.940	3.699	1.00 35.59	D
ATOM	3662	N	GLU		85	104.401	38.599	5.327	1.00 34.09	D
	3663	CA	GLU		85	103.695	39.561	4.489	1.00 32.99	Ð
ATOM								4.939	1.00 35.56	D
MOTA	3664	CB	GLU		85	102.239	39.714			D
MOTA	3665	CG	GLU		85	101.370	38.475	4.746	1.00 40.80	
MOTA	3666	CD	GLU	D	85	101.019	38.215	3.291	1.00 43.32	D
MOTA	3667	OE1	GLU	D	85	100.409	39.104	2.658	1.00 46.21	D
ATOM	3668	OE2	GLU	D	85	101.345	37.119	2.782	1.00 44.58	D
ATOM	3669	C	GLU		85	104.418	40.886	4.681	1.00 31.21	D
	3670	0	GLU		85	105.220	41.024	5.602	1.00 32.36	D
ATOM								3.808	1.00 29.71	D
MOTA	3671	N	VAL		86	104.140	41.848			D
ATOM	3672	CA	VAL			104.749	43.170	3.882	1.00 27.94	_
MOTA	3673	CB	VAL	D	86	105.079	43.712	2.467	1.00 26.90	D
MOTA	3674	CG1	VAL	D	86	105.569	45.166	2.543	1.00 23.11	D
ATOM	3675	CG2	VAL	D	86	106.134	42.829	1.821	1.00 24.31	Ð
ATOM	3676	C	VAL		86	103.767	44.114	4.574	1.00 29.81	D
	3677	0	VAL		86	102.658	44.343	4.088	1.00 30.28	D
ATOM								5.729	1.00 29.08	D
MOTA	3678	N	PRO		87	104.162	44.666			
ATOM	3679	CD	PRO		87	105.356	44.310	6.509	1.00 29.37	D
ATOM	3680	CA	PRO	D	87	103.306	45.583	6.485	1.00 30.85	D
MOTA	3681	CB	PRO	D	87	104.083	45.791	7.786	1.00 30.80	D
MOTA	3682	CG	PRO	D	87	104.878	44.551	7.920	1.00 30.83	D
ATOM	3683	C	PRO		87	103.049	46.907	5.772	1.00 31.43	D
	3684	0	PRO		87	103.863	47.357	4.968	1.00 31.78	D
ATOM									1.00 31.85	D
MOTA	3685	N	GLU		88	101.907	47.517	6.081		
MOTA	3686	CA	GLU		88	101.516	48.808	5.521	1.00 32.77	D
MOTA	3687	CB	GLU	D	88	100.195	48.687	4.744	1.00 35.18	D
MOTA	3688	CG	GLU	D	88	99.814	49.960	3.987	1.00 43.00	D
MOTA	3689	CD	GLU	D	88	98.512	49.839	3.205	1.00 46.30	D
ATOM	3690	OE1			88	97.439	49.745	3.837	1.00 47.40	D
ATOM	3691	OE2			88	98.564	49.840	1.954	1.00 48.25	D
							49.748	6.721	1.00 31.26	D
MOTA	3692	C	GLU		88	101.338				D
ATOM	3693	0	GLU		88	100.556	49.457	7.630	1.00 31.21	
MOTA	3694	N	VAL	D	89	102.060	50.864	6.728	1.00 28.43	D
MOTA	3695	CA	VAL	D	89	101.988	51.806	7.842	1.00 26.87	D

ATOM	3696	СВ	VAL :	D	89	103.385	52.024	8.454	1.00 26.58	D
			VAL :		89	103.277	52.886	9.699	1.00 26.80	D
ATOM	3697	CG1								D
MOTA	3698	CG2	VAL :		89	104.021	50.679	8.787	1.00 24.58	
ATOM	3699	C	VAL	D	89	101.389	53.174	7.505	1.00 27.02	D
ATOM	3700	0	VAL	D	89	101.698	53.772	6.473	1.00 26.22	D
MOTA	3701	N	THR	D	90	100.530	53.662	8.394	1.00 26.33	D
ATOM	3702	CA	THR	מ	90	99.881	54.955	8.219	1.00 26.05	D
	3703	CB	THR		90	98.414	54.802	7.769	1.00 27.24	D
ATOM									1.00 31.41	D
MOTA	3704	OG1	THR		90	98.359	54.063	6.543		
ATOM	3705	CG2	THR	D	90	97.786	56.163	7.545	1.00 28.57	D
ATOM	3706	C	THR	D	90	99.883	55.698	9.546	1.00 24.83	D
ATOM	3707	0	THR	D	90	99.542	55.120	10.581	1.00 25.45	D
ATOM	3708	N	VAL		91	100.266	56.972	9.512	1.00 22.04	D
		CA	VAL		91	100.300	57.791	10.716	1.00 21.50	D
ATOM	3709							11.031	1.00 23.04	D
MOTA	3710	CB	VAL		91	101.749	58.280			
ATOM	3711	CG1	VAL	D	91	101.737	59.245	12.225	1.00 22.74	D
MOTA	3712	CG2	VAL	D	91	102.650	57.082	11.340	1.00 20.38	D
MOTA	3713	C	VAL	D	91	99.369	58.993	10.553	1.00 21.65	D
ATOM	3714	0	VAL	D	91	99.357	59.653	9.509	1.00 21.70	D
ATOM	3715	N		D	92	98.573	59.252	11.586	1.00 21.34	D
						97.633	60.363	11.580	1.00 21.48	D
MOTA	3716	CA		D -	92					D
ATOM	3717	CB	PHE	D	92	96.370	59.985	10.788	1.00 21.60	
MOTA	3718	CG	PHE	D	92	95.652	58.771	11.314	1.00 22.22	D
MOTA	3719	CD1	PHE	D	92	94.601	58.902	12.215	1.00 24.10	Ð
ATOM	3720	CD2	PHE	D	92	96.038	57.495	10.925	1.00 24.53	D
ATOM	3721	CE1		D	92	93.940	57.774	12.724	1.00 22.72	D
						95.386	56.355	11.428	1.00 23.87	D
ATOM	3722	CE2	PHE		92				1.00 21.18	D
MOTA	3723	CZ	PHE		92	94.335	56.501	12.329		
ATOM	3724	С	PHE	D	92	97.303	60.700	13.030	1.00 22.72	D
ATOM	3725	0	PHE	D	92	97.607	59.921	13.933	1.00 22.31	D
MOTA	3726	N	SER	D	93	96.696	61.859	13.261	1.00 22.45	D
ATOM	3727	CA	SER		93	96.366	62.262	14.623	1.00 21.69	D
		CB	SER		93	96.599	63.764	14.799	1.00 20.96	D
MOTA	3728							14.010	1.00 25.08	D
MOTA	3729	OG	SER		93	95.696	64.508			
MOTA	3730	C	SER	D	93	94.931	61.913	14.990	1.00 21.02	D
ATOM	3731	0	SER	D	93	94.078	61.755	14.127	1.00 20.62	D
MOTA	3732	N	LYS	D	94	94.676	61.791	16.283	1.00 20.66	D
ATOM	3733	CA	LYS	D	94	93.350	61.453	16.768	1.00 24.11	D
ATOM	3734	CB	LYS		94	93.444	60.985	18.223	1.00 24.91	D
					94	92.121	60.605	18.865	1.00 29.49	D
ATOM	3735	CG	LYS						1.00 32.97	D
ATOM	3736	CD	LYS		94	92.353	60.101	20.293		
MOTA	3737	CE	LYS	D	94	91.050	59.909	21.052	1.00 33.37	D
MOTA	3738	NZ	LYS	D	94	90.175	58.897	20.399	1.00 34.08	D
ATOM	3739	С	LYS	D	94	92.406	62.646	16.654	1.00 24.40	D
ATOM	3740	0	LYS	D	94	91.224	62.495	16.356	1.00 24.55	D
ATOM	3741	N	SER		95	92.935	63.834	16.894	1.00 25.54	D
					95	92.133	65.040	16.815	1.00 29.22	D
MOTA	3742	CA	SER					18.208	1.00 30.47	D
MOTA	3743	CB	SER		95	91.932	65.643			
ATOM	3744	OG	SER	D	95	91.236	64.746	19.060	1.00 36.11	D
ATOM	3745	C	SER	D	95	92.843	66.046	15.932	1.00 29.71	D
MOTA	3746	0	SER	D	95	93.993	65.834	15.531	1.00 29.68	D
ATOM	3747	N	PRO	D	96	92.159	67.146	15.588	1.00 29.93	D
ATOM	3748	CD	PRO	D	96	90.760	67.532	15.843	1.00 31.14	D
	3749	CA	PRO		96	92.836	68.129	14.747	1.00 29.29	D
ATOM							69.097	14.369	1.00 31.65	D
ATOM	3750	CB	PRO		96	91.714				D
MOTA	3751	CG	PRO	D	96	90.777	69.010	15.545	1.00 30.66	
MOTA	3752	C	PRO	D	96	93.939	68.765	15.587	1.00 27.35	D
MOTA	3753	0	PRO	D	96	93.818	68.904	16.806	1.00 24.86	D
ATOM	3754	N	VAL	D	97	95.025	69.127	14.929	1.00 26.81	D
ATOM	3755	CA	VAL		97	96.158	69.706	15.615	1.00 29.25	D
					97	97.438	69.501	14.783	1.00 31.49	D
ATOM	3756	CB	VAL				69.998	15.556	1.00 33.50	D
MOTA	3757	CG1			97	98.652				
ATOM	3758	CG2	VAL	D	97	97.583	68.029	14.415	1.00 34.03	D
ATOM	3759	C	VAL	D	97	96.007	71.196	15.910	1.00 28.80	D
ATOM	3760	0	VAL	\mathfrak{D}	97	95.749	71.998	15.012	1.00 28.78	D
ATOM	3761	N	THR		98	96.144	71.559	17.178	1.00 27.47	D
ATOM	3762	CA	THR		98	96.091	72.960	17.572	1.00 26.55	D
					98	94.723	73.365	18.209	1.00 26.16	D
ATOM	3763	CB	THR					19.575	1.00 31.83	D
MOTA	3764	OG3			98	94.684	72.961			
MOTA	3765	CG2			98	93.567	72.717	17.469	1.00 23.66	D
MOTA	3766	C	THR	D	98	97.220	73.114	18.581	1.00 25.73	D
MOTA	3767	0	THR	D	98	97.260	72.412	19.591	1.00 27.12	D
ATOM	3768	N	LEU	D	99	98.159	74.005	18.285	1.00 26.12	D
ATOM	3769	CA	LEU		99	99.307	74.236	19.156	1.00 27.47	D
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ATOM	3770	CB	LEU D	99	100.089	75.459	18.675	1.00 31.04	D
ATOM	3771	CG	LEU D	99	100.758	75.309	17.310	1.00 33.09	D
ATOM	3772	CD1	rea D	99	101.458	76.607	16.940	1.00 36.20	D
ATOM	3773	CD2	LEU D	99	101.754	74.165	17.361	1.00 35.56	D
ATOM	3774	C	LEU D	99	98.935	74.416	20.621	1.00 26.08	D
ATOM	3775	0	LEU D	99	98.077	75.222	20.946	1.00 25.97	D
ATOM	3776	N	GLY D	100	99.585	73.654	21.500	1.00 26.97	D D
ATOM	3777	CA	GLY D	100	99.310	73.749	22.924	1.00 26.03 1.00 26.02	D D
ATOM	3778	C	GLY D	100	98.233	72.798 72.662	23.422 24.629	1.00 26.02 1.00 25.51	D
ATOM	3779	O	GLY D	100 101	98.020 97.553	72.062	22.491	1.00 25.73	D
ATOM	3780 3781	N CA	GLN D	101	96.490	71.199	22.820	1.00 28.13	D
ATOM ATOM	3782	CB		101	95.372	71.297	21.776	1.00 32.24	D
ATOM	3783	CG	GLN D	101	94.617	69.981	21.560	1.00 38.65	D
ATOM	3784	CD	GLN D	101	94.680	69.459	20.115	1.00 41.08	D
ATOM	3785	OE1	GLN D	101	95.760	69.348	19.511	1.00 38.18	D
ATOM	3786	NE2	GLN D	101	93.515	69.119	19.566	1.00 40.87	D
ATOM	3787	C	GLN D	101	96.994	69.756	22.861	1.00 25.22	D
ATOM	3788	0	GLN D	101	97.477	69.245	21.857	1.00 24.55	D
ATOM	3789	N	PRO D	102	96.885	69.078	24.019	1.00 24.18	D
ATOM	3790	CD	PRO D		96.436	69.544	25.343	1.00 22.22	D
MOTA	3791	CA	PRO D		97.359	67.683	24.080	1.00 22.76	D
ATOM	3792	CB	PRO D	102	96.983	67.253	25.494	1.00 22.02	D D
MOTA	3793	CG	PRO D		97.088	68.542	26.274 23.015	1.00 22.44 1.00 21.72	D
ATOM	3794	C	PRO D		96.649	66.845 66.922	23.015	1.00 21.72	D
ATOM	3795	0	PRO D	102 103	95.429 97.409	66.055	22.264	1.00 19.84	D
ATOM	3796 3797	N CA	ASN D		96.833	65.225	21.209	1.00 17.89	D
ATOM ATOM	3798	CB		103	97.112	65.856	19.838	1.00 16.30	D
ATOM	3799	CG	ASN D		96.005	65.587	18.824	1.00 16.50	D
ATOM	3800	OD1		103	95.552	64.446	18.636	1.00 16.80	D
ATOM	3801	ND2			95.569	66.643	18.160	1.00 14.61	D
ATOM	3802	C		103	97.410	63.805	21.248	1.00 17.24	D
ATOM	3803	0	ASN D	103	98.199	63.473	22.129	1.00 15.74	D
ATOM	3804	N	ILE D	104	97.010	62.977	20.284	1.00 17.39	D
ATOM	3805	CA	ILE D	104	97.465	61.595	20.198	1.00 15.30	D
MOTA	3806	CB	ILE D	104	96.402	60.627	20.755	1.00 17.89	D
MOTA	3807	CG2	ILE D		96.818	59.175	20.498	1.00 13.27	D
ATOM	3808	CG1			96.202	60.886	22.253	1.00 18.46	D
ATOM	3809	CD1			95.179	59.965	22.895	1.00 17.98 1.00 17.15	Ð D
ATOM	3810	C	ILE D		97.760	61.185 61.283	18.763 17.902	1.00 17.15	D
MOTA	3811	O	LEU D		96.887 98.987	60.727	18.509	1.00 16.66	D
ATOM	3812 3813	N CA	LEU D		99.370	60.272	17.177	1.00 16.59	D
ATOM ATOM	3814	CB	LEU D		100.864	60.482	16.895	1.00 17.56	D
ATOM	3815	CG	LEU D		101.375	61.926	16.842	1.00 21.66	D
ATOM	3816	CD1			102.811	61.943	16.302	1.00 21.26	D
ATOM	3817	CD2		105	100.460	62.771	15.951	1.00 21.56	D
ATOM	3818	С	LEU D	105	99.061	58.804	17.128	1.00 17.13	D
MOTA	3819	0	LEU D	105	99.368	58.056	18.056	1.00 18.35	D
ATOM	3820	N	ILE D	106	98.432	58.399	16.039	1.00 17.88	D
ATOM	3821	CA	ILE D	106	98.045	57.016	15.839	1.00 17.14	D
ATOM	3822	CB	ILE D		96.525	56.939	15.492	1.00 16.99	D D
ATOM	3823	CG2			96.093	55.496 57.619	15.318 16.604	1.00 15.63 1.00 19.04	D
ATOM	3824	CG1			95.711 94.238	57.877	16.260	1.00 15.04	D
ATOM	3825	CD1	ILE D		98.876	56.431	14.700	1.00 17.19	D
MOTA MOTA	3826 3827	0	ILE D		98.941	57.004	13.618	1.00 16.06	D
ATOM	3828	N	CYS D		99.540	55.312	14.966	1.00 18.84	D
ATOM	3829	CA	CYS I		100.339	54.637	13.954	1.00 19.74	D
ATOM	3830	C	CYS I		99.634	53.323	13.670	1.00 20.17	D
MOTA	3831	0	CYS I		99.632	52.421	14.507	1.00 20.08	D
ATOM	3832	CB	CYS I	107	101.755	54.349	14.453	1.00 22.00	D
ATOM	3833	SG	CYS I	107	102.800	53.514	13.211	1.00 28.61	D
MOTA	3834	N	LEU I	108	99.027	53.221	12.493	1.00 19.48	D
ATOM	3835	CA	LEU I	108	98.313	52.015	12.113	1.00 19.67	D
MOTA	3836	CB	LEU I		97.024	52.391	11.369	1.00 19.98	D
MOTA	3837	CG	LEU I		95.977	51.358	10.925	1.00 20.40	D
ATOM	3838	CD:			95.883	51.366	9.412	1.00 20.15	D D
MOTA	3839	CD:			96.301	49.971	11.454	1.00 19.44 1.00 19.84	D D
MOTA	3840	C	LEU I		99.207 99.657	51.145 51.563	11.237 10.170	1.00 19.84	D
MOTA	3841	O M	LEU I		99.657	49.940	11.721	1.00 20.11	D
MOTA MOTA	3842 3843	N CA	VAL I		100.289	48.972	11.016	1.00 19.64	D
WT OIL	2042	CM	A 42771 T	الت الماسات ال	2001202				

MOTA	3844	CB	VAL	D	109	10	1.368	4	8.402	13	L.958	1.0	00	19.40	D	
ATOM	3845	CGl	VAL	D	109	10	2.290	4	7.474	13	1.202	1.0	00	18.01	D	
ATOM	3846	CG2	VAL	D	109	10	2.155	4	9.560	12	2.590	1.0	00	17.30	D	
ATOM	3847	C	VAL	D	109	9	99.321	4	7.876	10	0.568	1.0	00	21.45	D	
ATOM	3848	0	VAL				8.845	4	7.079	13	1.382	1.0	00	22.65	D	
ATOM	3849	N			110		99.022		7.861		9.274	1.0	00	22.00	D	
ATOM	3850	CA	ASP				98.086		6.901		3.689			23.80	D	
		CB			110		97.156		7.648		7.728			24.68	D	
ATOM	3851										7.603			26.64	D	
ATOM	3852	CG	ASP				95.790		17.002							
MOTA	3853	OD1	ASP				95.582		15.915		3.177			28.80	D	
ATOM	3854	OD2	ASP				94.920		17.591		5.926			27.99	D	
ATOM	3855	C	ASP	D	110		98.802		15.756		7.944			23.77	D	
ATOM	3856	0	ASP	D	110	10	00.005	4	15.831		7.684			22.82	D	
ATOM	3857	N	ASN	D	111	2	98.044	4	4.711	,	7.604	1.0	00	23.55	D	
MOTA	3858	CA	ASN	D	111	9	98.548	4	13.530	6	5.889	1.0	00	23.79	D	
ATOM	3859	CB	ASN	D	111	9	98.880	4	13.867	Ĭ	5.425	1.	00	25.36	D	
ATOM	3860	CG	ASN	D	111	9	99.079	4	12.610	4	4.562	1.0	00	29.95	D	
ATOM	3861	OD1	ASN	D	111	9	99.981	4	12.547		3.724	1.0	00	29.58	D	
ATOM	3862	ND2			111	g	98.220	4	1.611	4	4.761	1.0	00	30.51	D	
ATOM	3863	C	ASN				99.786		12.941		7.556			22.70	D	
		0	ASN				00.834		12.784		6.929			22.97	D	
MOTA	3864								12.612		8.835			22.14	D	
ATOM	3865	N	ILE		112		99.656								D	
ATOM	3866	CA	ILE		112		00.754		12.038		9.598			20.20		
MOTA	3867	CB			112		00.746		12.536		1.055			18.82	D	
ATOM	3868	CG2	ILE	D	112	10	01.926		1.950		1.808			15.77	D	
ATOM	3869	CG1	ILE	D	112	10	00.770	4	14.058	1:	1.103			19.09	D	
ATOM	3870	CD1	ILE	D	112	10	00.630	4	14.602	1:	2.514	1.	00	21.18	D	
MOTA	3871	С	ILE	D	112	10	00.666	4	10.512		9.659	1.	00	21.41	D	
ATOM	3872	0	ILE	D	112	9	99.626	3	39.960	1	0.002	1.	00	22.04	D	
ATOM	3873	N	PHE	D	113	10	01.765	3	39.838		9.338	1.	00	21.35	ם	
ATOM	3874	CA	PHE			10	01.818	3	38.386	(9.409	1.	00	19.93	D	
ATOM	3875	CB			113		00.822		37.726		8.462	1.	00	21.28	D	
	3876	CG			113		00.537		36.306		8.825			20.91	D	
ATOM			PHE				99.630		36.012		9.838			19.85	D	
ATOM	3877	CD1									8.230			22.61	D	
MOTA	3878	CD2			113		01.244		35.261						D	
ATOM	3879	CE1			113		99.430		34.698		0.264			20.63		
ATOM	3880	CE2			113		01.054		33.942		8.646	1.		21.21	D	
ATOM	3881	CZ	PHE	D	113		00.144		33.660		9.669			20.87	D	
MOTA	3882	C	PHE	D	113	10	03.201	3	37.871		9.071			19.98	D	
ATOM	3883	0	PHE	D	113	1	03.762	3	38.238		8.044	1.	00	20.80	D	
ATOM	3884	N	PRO	D	114	1	03.765		37.005		9.925	1.	00	21.26	D	
ATOM	3885	CD.	PRO	D	114	1	05.101	:	36.414		9.732	1.	00	21.94	D	
ATOM	3886	CA	PRO	D	114	1	03.150		36.518	1	1.166	1.	00	21.41	D	
ATOM	3887	CB	PRO	D	114	1	04.117	:	35.424	1	1.625	1.	00	21.03	D	
ATOM	3888	CG	PRO	D	114	1	05.441	•	35.912	1	1.115	1.	00	22.98	D	
ATOM	3889	C			114	1	03.002		37.648	1	2.185	1.	00	21.84	D	
ATOM	3890	Ō			114		03.621		38.711		2.034	1.	00	20.41	D	
MOTA	3891	N			115		02.167		37.441		3.222			22.52	D	
		CD			115		01.314		36.256		3.445			22.08	D	
ATOM	3892						01.937		38.448		4.266			21.19	D	
ATOM	3893	CA			115						5.025			20.92	D	
ATOM	3894	CB			115		00.730		37.895						D	
ATOM	3895	CG			115		00.917		36.410		4.902			19.88		
MOTA	3896	C			115		03.139		38.683		5.171			21.62	D	
ATOM	3897	0	PRO	D	115		03.127		38.336		6.356			22.92	D	
MOTA	3898	N	VAL	D	116	1	04.179		39.263		4.588			21.58	D	
ATOM	3899	CA	VAL	D	116	1	05.405		39.598	1	5.300	1.	00	22.53	D	
MOTA	3900	CB	VAL	\mathfrak{D}	116	1	06.520		38.554	1	5.067	1.	00	24.90	D	
MOTA	3901	CG1	VAL	D	116	1	07.817	,	39.035	1	5.713	1.	00	24.06	D	t
ATOM	3902	CG2	VAL	D	116	1	06.104		37.195	1	5.641	1.	00	24.88	D	ı
ATOM	3903	C			116	1	.05.855		40.929	1	4.708	1.	00	21.86	. D	,
ATOM	3904	0			116	1	06.114		41.027	1	3.509	1.	00	20.87	D)
ATOM	3905	N			117	1	05.935	,	41.962	1	5.534	1.	00	20.65	D)
					117		.06.338		43.255		5.007		00		D	,
MOTA	3906	CA			117		.05.126		43.233 43.978		4.345			18.11	D	
ATOM	3907	CB					.04.156		44.473		.5.403		00		D	
ATOM	3908	CG1											00		D	
ATOM	3909	CG2			117		.05.599		45.101		.3.469				D	
ATOM	3910	C			117		.06.928		44.137		.6.092			23.84		
MOTA	3911	0			117		.06.677		43.936		.7.280			24.78	D	
ATOM	3912	N			118		.07.719		45.113		.5.670			27.93	D	
MOTA	3913	CA	ASN	D	118		.08.348		46.051		.6.593			30.45	D	
ATOM	3914	CB	ASN	D	118		.09.866		45.898	3 1	6.538			33.93	D	
ATOM	3915	CG	ASN	D	118	1	10.564	Į.	46.644	. 1	7.650			39.88	D	
ATOM	3916	OD I	L ASN	D	118	1	.10.327	7	47.834	. 1	7.856	1.	.00	42.45		
MOTA	3917	ND2	asn	D	118	3	11.438	3	45.946	; 1	L8.375	1.	.00	43.14	D)

ATOM	3918	C	ASN D	118	107.960	47.465	16.181	1.00 27.72	D
ATOM	3919	0			108.398	47.952	15.140	1.00 26.88	D D
ATOM	3920	N		119	107.126 106.680	48.113 49.476	16.988 16.700	1.00 27.59 1.00 27.12	D
ATOM ATOM	3921 3922	CA CB	ILE D	119 119	105.133	49.580	16.719	1.00 27.12	D
ATOM	3923	CG2	ILE D	119	104.698	50.994	16.346	1.00 26.16	D
ATOM	3924	CG1	ILE D	119	104.528	48.572	15.741	1.00 24.63	D
ATOM	3925	CD1	ILE D	119	103.026	48.423	15.877	1.00 24.19	D
ATOM	3926	C	ILE D	119	107.243	50.436	17.746	1.00 27.72	D
MOTA	3927	0	ILE D	119	107.050	50.248	18.946	1.00 26.86	D
ATOM	3928	N	THR D	120	107.951	51.460 52.423	17.291 18.214	1.00 27.54 1.00 29.37	D D
ATOM	3929	CA CB	THR D	120 120	108.524 110.022	52.423	18.477	1.00 25.37	D
ATOM ATOM	3930 3931	OG1			110.722	52.034	17.229	1.00 35.14	D
ATOM	3932	CG2		120	110.176	50.817	19.247	1.00 35.67	D
MOTA	3933	C	THR D	120	108.369	53.826	17.668	1.00 27.95	D
ATOM	3934	0	THR D	120	108.398	54.035	16.459	1.00 29.89	D
MOTA	3935	N	TRP D		108.187	54.789	18.560	1.00 26.28	D
MOTA	3936	CA	TRP D		108.031	56.171	18.135 18.940	1.00 26.93 1.00 24.20	D D
ATOM	3937	CB	TRP D		106.935 105.568	56.866 56.343	18.687	1.00 24.20	D
ATOM ATOM	3938 3939	CG CD2			104.643	56.826	17.707	1.00 20.30	D
ATOM	3940	CE2			103.454	56.085	17.856	1.00 20.70	D
ATOM	3941	CE3			104.705	57.817	16.717	1.00 17.15	D
MOTA	3942	CD1	TRP D	121	104.929	55.351	19.365	1.00 21.06	D
ATOM	3943	NE1	TRP D	121	103.655	55.190	18.875	1.00 22.39	D
MOTA	3944	CZ2			102.332	56.305	17.057	1.00 17.25	D D
ATOM	3945	CZ3			103.593	58.036 57.282	15.924 16.099	1.00 17.92 1.00 19.11	D
ATOM	3946	CH2 C	TRP D		102.419 109.319	56.957	18.284	1.00 26.88	D
ATOM ATOM	3947 3948	0	TRP D		110.059	56.789	19.251	1.00 27.48	D
ATOM	3949	N	LEU D		109.572	57.830	17.321	1.00 29.82	D
ATOM	3950	CA	LEU D	122	110.764	58.658	17.343	1.00 31.91	D
ATOM	3951	CB	LEU D	122	111.664	58.331	16.144	1.00 34.65	D
ATOM	3952	CG	LEU D		112.391	56.977	16.112	1.00 37.28	D
ATOM	3953	CD1			113.247	56.828 55.840	17.360 16.025	1.00 37.11 1.00 39.41	D D
MOTA	3954 3955	CD2 C	LEU D		111.394 110.416	60.142	17.324	1.00 33.11	D
ATOM ATOM	3956	0	LEU D		109.619	60.593	16.503	1.00 31.46	D
ATOM	3957	N	SER D		111.010	60.889	18.250	1.00 31.03	D
ATOM	3958	CA	SER D	123	110.813	62.331	18.326	1.00 33.04	D
MOTA	3959	CB	SER D	123	110.312	62.745	19.712	1.00 32.42	D
MOTA	3960	OG	SER D		110.169	64.154	19.793 18.062	1.00 32.43 1.00 33.10	D D
ATOM	3961	C	SER D		112.184 113.108	62.948 62.784	18.860	1.00 33.10	D
ATOM ATOM	3962 3963	N		124	112.309	63.646	16.941	1.00 33.51	D
ATOM	3964	CA	ASN D		113.575	64.258	16.553	1.00 36.20	D
ATOM	3965	CB	ASN D	124	113.963	65.392	17.510	1.00 34.61	D
ATOM	3966	CG	ASN D		112.946	66.512	17.531	1.00 34.17	D
ATOM	3967		L ASN I		112.262	66.764	16.539	1.00 34.73 1.00 35.34	D D
MOTA	3968		2 ASN D		112.850 114.664	67.202 63.191	18.660 16.561	1.00 35.34	D
ATOM ATOM	3969 3970	C O	ASN I		115.747	63.401	17.104	1.00 37.93	D
ATOM	3971	Ŋ	GLY I		114.358	62.039	15.970	1.00 38.73	D
ATOM	3972	CA	GLY I		115.317	60.951	15.910	1.00 39.56	D
MOTA	3973	C	GLY I	125	115.457	60.131	17.183	1.00 40.55	D
ATOM	3974	0	GLY I		116.051	59.054	17.157	1.00 42.52	Ð
MOTA	3975	N	HIS I		114.911	60.622	18.291	1.00 40.35 1.00 41.15	D D
ATOM	3976	CA	HIS I		115.009 115.234	59.918 60.923	19.569 20.702	1.00 43.51	, D
ATOM ATOM	3977 3978	CB CG	HIS I		116.525	61.678	20.702	1.00 47.67	D
ATOM	3979		HIS I		116.775	62.997	20.422	1.00 47.36	D
MOTA	3980		l HIS I		117.757	61.064	20.694	1.00 49.39	D
ATOM	3981		1 HIS I		118.709	61.973	20.581	1.00 48.59	D
MOTA	3982		2 HIS I		118.140	63.154	20.415	1.00 48.17	D
ATOM	3983	C		126	113.794		19.907	1.00 40.38 1.00 39.87	D D
ATOM	3984	0	HIS I		112.648 114.056	59.458 57.863	19.706 20.438	1.00 39.87	D
ATOM ATOM	3985	N CV	SER I		112.995	56.939	20.436	1.00 39.54	D
ATOM ATOM	3986 3987	CA CB	SER I		113.592		21.232	1.00 40.04	D
MOTA	3988	OG	SER I		114.299		20.159	1.00 45.08	D
ATOM	3989	C	SER I		112.167		21.979	1.00 38.18	D
MOTA	3990	0	SER I		112.707		22.930		D D
MOTA	3991	N	VAL I	D 128	110.854	57.326	21.894	1.00 36.40	ע
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ATOM	3992	CA	VAL D 128	109.967	57.800	22.942	1.00 35.00	D
ATOM	3993	CB	VAL D 128	108.699 107.834	58.444 59.001	22.358 23.479	1.00 33.68 1.00 32.31	D D
MOTA MOTA	3994 3995	CG1 CG2	VAL D 128 VAL D 128	107.834	59.543	21.383	1.00 32.51	D
MOTA	3996	C	VAL D 128	109.574	56.608	23.790	1.00 34.62	D
ATOM	3997	0	VAL D 128	109.150	55.584	23.268	1.00 35.98	D
ATOM	3998	N	THR D 129	109.715	56.743	25.100	1.00 35.57	D
ATOM	3999	CA	THR D 129	109.393	55.653	26.007	1.00 38.21 1.00 40.63	D D
ATOM	4000	CB	THR D 129 THR D 129	110.562 110.184	55.410 54.413	26.992 27.949	1.00 44.78	D
ATOM ATOM	4001 4002	OG1 CG2	THR D 129	110.929	56.700	27.715	1.00 42.66	D
ATOM	4003	Ç	THR D 129	108.103	55.862	26.799	1.00 36.54	D
ATOM	4004	0	THR D 129	107.359	54.911	27.042	1.00 38.87	D
ATOM	4005	N	GLU D 130	107.833	57.101	27.195	1.00 33.00 1.00 31.03	D ·
ATOM	4006	CA CB	GLU D 130 GLU D 130	106.631 106.935	57.401 58.453	27.963 29.039	1.00 31.03	D
ATOM ATOM	4007 4008	CG	GLU D 130	108.067	58.089	29.987	1.00 38.08	D
ATOM	4009	CD	GLU D 130	107.809	56.788	30.731	1.00 43.43	D
MOTA	4010	OE1	GLU D 130	106.744	56.672	31.375	1.00 45.61	D
MOTA	4011	OE2	GLU D 130	108.671	55.879	30.675	1.00 45.67	D D
ATOM	4012	C	GLU D 130	105.521 105.795	57.922 58.527	27.058 26.029	1.00 27.87 1.00 24.56	D
MOTA MOTA	4013 4014	N	GLU D 130 GLY D 131	104.272	57.692	27.457	1.00 26.29	D
ATOM	4015	CA	GLY D 131	103.140	58.166	26.679	1.00 25.19	D
ATOM	4016	C	GLY D 131	102.826	57.304	25.474	1.00 24.46	D
MOTA	4017	0	GLY D 131	102.130	57.725	24.559	1.00 23.65	D
ATOM	4018	N	VAL D 132	103.349	56.089	25.476 24.379	1.00 22.83 1.00 23.04	D D
ATOM	4019	CA	VAL D 132 VAL D 132	103.117 104.448	55.169 54.674	23.784	1.00 23.04	D
ATOM ATOM	4020 4021	CB CG1		104.182	53.538	22.821	1.00 24.12	D
ATOM	4022	CG2		105.164	55.816	23.076	1.00 22.85	D
ATOM	4023	C	VAL D 132	102.326	53.943	24.829	1.00 21.91	D
MOTA	4024	0	VAL D 132	102.535	53.416	25.917	1.00 21.27 1.00 22.08	D D
MOTA	4025	N	SER D 133	101.412 100.622	53.499 52.307	23.979 24.251	1.00 22.08	D
ATOM ATOM	4026 4027	CA CB	SER D 133 SER D 133	99.405	52.637	25.119	1.00 21.95	D
ATOM	4028	OG	SER D 133	98.567	53.595	24.498	1.00 27.01	D
ATOM	4029	C	SER D 133	100.178	51.738	22.908	1.00 21.27	D
MOTA	4030	0	SER D 133	100.344	52.369	21.864	1.00 19.82	D D
ATOM	4031	N	GLU D 134	99.627 99.182	50.538 49.938	22.926 21.689	1.00 20.29 1.00 24.12	D
ATOM ATOM	4032 4033	CA CB	GLU D 134 GLU D 134	100.370	49.323	20.932	1.00 26.01	D
ATOM	4034	CG	GLU D 134	100.932	48.045	21.532	1.00 30.80	D
MOTA	4035	CD	GLU D 134	102.080	47.480	20.704	1.00 35.43	D
MOTA	4036	OE1		102.273	46.243	20.702	1.00 36.93 1.00 37.66	D D
ATOM	4037	OE2		102.793 98.127	48.278 48.882	20.057 21.955	1.00 37.88	D
ATOM ATOM	4038 4039	С 0	GLU D 134 GLU D 134	97.968	48.416	23.081	1.00 22.94	D
ATOM	4040	N	THR D 135	97.400	48.522	20.908	1.00 21.95	D
MOTA	4041	CA	THR D 135	96.361	47.519	21.009	1.00 20.78	D
ATOM	4042	CB	THR D 135	95.368	47.625	19.843	1.00 20.82 1.00 22.24	D D
ATOM	4043	OG1		96.032 94.833	47.262 49.046	18.623 19.721	1.00 22.24	D
ATOM ATOM	4044 4045	CG2 C	THR D 135	97.037	46.168	20.890	1.00 20.80	D
ATOM	4046	0	THR D 135	98.259	46.084	20.742	1.00 21.08	D
ATOM	4047	N	SER D 136	96.234	45.116	20.972	1.00 19.11	D
ATOM	4048	CA	SER D 136	96.728	43.764	20.790	1.00 16.93 1.00 19.17	D D
ATOM	4049	CB	SER D 136	95.769 95.656	42.755 42.951	21.428 22.831	1.00 19.17	D
MOTA	4050 4051	OG C	SER D 136 SER D 136	96.665	43.635	19.267	1.00 15.30	D
ATOM ATOM	4051	0	SER D 136	96.325	44.592	18.580	1.00 13.19	D
MOTA	4053	N	PHE D 137	97.002	42.472	18.733	1.00 16.43	D
MOTA	4054	CA		96.896			1.00 16.20	D
MOTA	4055	CB	PHE D 137	97.652			1.00 15.86 1.00 17.29	D D
ATOM	4056		PHE D 137 1 PHE D 137	99.138 99.792			1.00 17.23	D
MOTA MOTA	4057 4058	CD:		99.894			1.00 17.79	D
ATOM	4058			101.187			1.00 21.20	D
ATOM	4060		2 PHE D 137	101.291				D
ATOM	4061			101.935				D D
MOTA	4062		PHE D 137	95.402 94.823		_		D D
MOTA MOTA	4063 4064		PHE D 137 LEU D 138	94.823				D
MOTA	4064			93.367				D

ATOM	4066	CB	LEU D	138	92.722	44.175	15.678	1.00 21.40	D
ATOM	4067	CG	LEU D	138	92.452	45.087	16.881	1.00 22.42	D
MOTA	4068	CD1	LEU D	138	91.889	44.277	18.032	1.00 23.38	D
MOTA	4069	CD2	LEU D	138	93.732	45.764	17.301	1.00 28.68	D
ATOM	4070	C	LEU D	138	93.230	41.982	14.593	1.00 20.56	D
ATOM	4071	0	LEU D	138	93.919	42.244	13.615	1.00 22.27	D
ATOM	4072	N	SER D	139	92.326	41.013	14.586	1.00 20.44	D
ATOM	4073	CA	SER D	139	92.143	40.142	13.427	1.00 19.23	D
ATOM	4074	CB	SER D	139	91.222	38.986	13.788	1.00 19.74	D
ATOM	4075	OG	SER D	139	89.888	39.443	13.861	1.00 21.32	D
ATOM	4076	C	SER D	139	91.594	40.802	12.168	1.00 19.43	D,
ATOM	4077	0	SER D	139	91.028	41.893	12.210	1.00 19.49	D
ATOM	4078	N	LYS D	140	91.755	40.102	11.050	1.00 18.62	D
ATOM	4079	CA	LYS D	140	91.276	40.553	9.749	1.00 19.20	D
ATOM	4080	CB	LYS D	140	92.437	41.058	8.895	1.00 18.92	D
ATOM	4081	CG	LYS D	1.40	93.286	42.126	9.554	1.00 19.38	D
ATOM	4082	CD	LYS D	140	93.254	43.393	8.758	1.00 20.95	D
ATOM	4083	CE	LYS D	140	93.833	43.195	7.377	1.00 18.23	D
	4084	NZ	LYS D	140	93.743	44.457	6.617	1.00 20.40	D
ATOM	4084	C	LYS D		90.660	39.339	9.068	1.00 19.16	D
MOTA		0	LYS D		91.091	38.217	9.312	1.00 19.77	D
MOTA	4086		SER D	141	89.670	39.552	8.207	1.00 21.60	D
ATOM	4087	N			89.030	38.438	7.507	1.00 23.19	D
ATOM	4088	CA	SER D		87.859	38.948	6.653	1.00 24.88	D
ATOM	4089	CB	SER D				5.655	1.00 28.69	D
MOTA	4090	OG ~	SER D		88.288	39.858 37.605	6.636	1.00 23.26	Đ
ATOM	4091	C	SER D		89.989		6.327	1.00 23.23	D
ATOM	4092	0	SER D		89.692	36.454	6.251	1.00 23.33	D
MOTA	4093	N	ASP D		91.137	38.159	5.429	1.00 22.54	D
MOTA	4094	CA		142	92.075	37.387	4.466	1.00 25.84	D
ATOM	4095	CB	ASP D		92.834	38.303		1.00 29.78	D
ATOM	4096	CG	ASP D		93.943	39.064	5.143	1.00 25.76	D
MOTA	4097	OD1			93.760	39.486	6.309	1.00 34.64	D
MOTA	4098	OD2		142	94.997	39.246	4.500		D
MOTA	4099	C	ASP D		93.045	36.637	6.336		D
MOTA	4100	0	ASP D		94.027	36.037	5.883	1.00 20.54	
ATOM	4101	$oldsymbol{N}_i$	HIS D		92.753	36.700	7.632	1.00 21.06	D
ATOM.	4102	CA	HIS D		93.522	36.020	8.659	1.00 19.58	D
MOTA	4103	CB	HIS D		93.628	34.534	8.317	1.00 19.03	D
MOTA	4104	CG	HIS D		92.295	33.892	8.104	1.00 23.00	D G
MOTA	4105	CD2	HIS D	143	91.827	33.108	7.104	1.00 24.78	D
MOTA	4106	ND1	HIS D	143	91.237	34.087	8.967	1.00 21.97	D
MOTA	4107	CE1	. HIS D	143	90.174	33.455	8.505	1.00 24.67	D
MOTA	4108	NE2	HIS D		90.504	32.853	7.375	1.00 24.72	D
MOTA	4109	C	HIS D	143	94.878	36.602	8.986	1.00 20.11	D
MOTA	4110	0	HIS D	143	95.691	35.962	9.654	1.00 21.09	D
MOTA	4111	N	SER D	144	95.118	37.820	8.514	1.00 21.24	D
ATOM	4112	CA	SER D	144	96.352	38.525	8.826	1.00 21.79	D
ATOM	4113	CB	SER D	144	96.834	39.353	7.627	1.00 20.33	D
MOTA	4114	OG	SER D	144	96.047	40.511	, 7.434	1.00 24.32	D
ATOM	4115	C	SER D	144	95.940	39.440	9.990	1.00 21.43	D
ATOM	4116	0	SER I	144	94.830	39.317	10.504	1.00 20.74	D
ATOM	4117	И	PHE I	145	96.809	40.352	10.412	1.00 21.56	D
ATOM	4118	CA	PHE I	145	96.463	41.235	11.523	1.00 22.54	D -
MOTA	4119	CB	PHE I	145	97.156	40.791	12.817	1.00 22.63	D
ATOM	4120	CG	PHE I	145	96.896	39.368	13.200	1.00 25.73	D
MOTA	4121	CDI	L PHE I	145	97.565	38.329	12.562	1.00 26.67	D -
MOTA	4122	CD2	PHE I	145	95.987	39.063	14.207	1.00 23.65	D
MOTA	4123	CEI	L PHE I	1.45	97.333	37.004	12.921	1.00 27.30	D
ATOM	4124	CE2	PHE I	145	95.750	37.746	14.572	1.00 25.43	D
MOTA	4125	CZ	PHE I	1.45	96.426	36.713	13.926	1.00 24.90	D
ATOM	4126	С	PHE I	145	96.850	42.687	11.299	1.00 22.51	D
ATOM	4127	0	PHE I	145	97.540	43.028	10.339	1.00 23.97	D
MOTA	4128	N	PHE I	146	96.371	43.540	12.198	1.00 20.96	D
ATOM	4129	CA	PHE I		96.729	44.946	12.190	1.00 19.68	D
ATOM	4130	CB	PHE I		95.696	45.817	11.439	1.00 17.70	D
MOTA	4131	CG	PHE I	146	94.392	46.041	12.159	1.00 15.76	D
ATOM	4132	CD:			94.201	47.173	12.948	1.00 16.08	D
ATOM	4133	CD:			93.321	45.170	11.976	1.00 14.70	D
ATOM	4134	CE:	_		92.961	47.442	13.543	1.00 13.47	D
ATOM	4135	CE:			92.080	45.426	12.563	1.00 15.43	D
MOTA	4136	CZ.		146	91.900	46.567	13.350	1.00 14.68	D
ATOM	4137		PHE 1		96.893	45.335		1.00 19.66	D
MOTA	4138		PHE 1		96.373	44.672		1.00 19.92	D
ATOM	4139	N		D 147	97.666	46.379	13.901	1.00 20.23	D
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ATOM	4140	CA	LYS D 147	97.910	46.817	15.260	1.00 19.84	Ð
ATOM	4141	СВ	LYS D 147	99.184	46.148	15.796	1.00 21.50	D
ATOM	4142	CG	LYS D 147	99.651	46.679	17.134	1.00 24.87	D
			LYS D 147	100.764	45.832	17.724	1.00 27.18	D
ATOM	4143	CD					1.00 31.41	D
MOTA	4144	CE	LYS D 147	100.220	44.515	18.253		
MOTA	4145	NZ	LYS D 147	101.086	43.984	19.341	1.00 32.97	D
ATOM	4146	C	LYS D 147	98.038	48.324	15.274	1.00 18.69	D
ATOM	4147	0	LYS D 147	98.603	48.914	14.352	1.00 20.14	D
ATOM	4148	N	ILE D 148	97.497	48.944	16.314	1.00 18.22	D
ATOM	4149	CA	ILE D 148	97.530	50.387	16.446	1.00 18.25	D
				96.092	50.942	16.548	1.00 20.80	D
MOTA	4150	CB	ILE D 148					D
ATOM	4151	CG2	ILE D 148	96.113	52.459	16.659		
MOTA	4152	CG1	ILE D 148	95.308	50.533	15.292	1.00 23.89	D
ATOM	4153	CD1	ILE D 148	93.840	50.858	15.314	1.00 24.42	D
ATOM	4154	C	ILE D 148	98.369	50.816	17.646	1.00 19.71	D
ATOM	4155	0	ILE D 148	98.213	50.294	18.757	1.00 17.77	D
ATOM	4156	N	SER D 149	99.284	51.753	17.395	1.00 19.08	D
			SER D 149	100.173	52.278	18.424	1.00 18.19	D
ATOM	4157	CA					1.00 18.51	D
ATOM	4158	CB	SER D 149	101.633	52.137	17.991		
ATOM	4159	OG	SER D 149	102.518	52.492	19.040	1.00 19.49	D -
ATOM	4160	C	SER D 149	99.839	53.744	18.646	1.00 18.14	D
ATOM	4161	0	SER D 149	99.591	54.490	17.693	1.00 18.17	D
ATOM	4162	N	TYR D 150	99.843	54.155	19.905	1.00 16.95	D
ATOM	4163	CA	TYR D 150	99.503	55.524	20.261	1.00 16.12	D
		CB	TYR D 150	98.310	55.524	21.213	1.00 15.57	D
ATOM	4164				54.750	20.701	1.00 16.81	D
ATOM	4165	CG	TYR D 150	97.116				D
ATOM	4166	CD1		96.291	55.276	19.709	1.00 14.33	
MOTA	4167	CE1	TYR D 150	95.197	54.554	19.222	1.00 17.50	D
ATOM	4168	CD2	TYR D 150	96.819	53.486	21.199	1.00 15.90	D
ATOM	4169	CE2	TYR D 150	95.731	52.760	20.719	1.00 18.41	D
ATOM	4170	CZ	TYR D 150	94.928	53.297	19.732	1.00 16.27	D
ATOM	4171	OH	TYR D 150	93.868	52.574	19.244	1.00 20.03	D
		C	TYR D 150	100.650	56.266	20.922	1.00 16.35	D
ATOM	4172			101.438	55.690	21.669	1.00 16.95	D
MOTA	4173	0	TYR D 150				1.00 16.64	D
MOTA	4174	N	LEU D 151	100.732	57.558	20.643		
ATOM	4175	$^{\mathrm{CA}}$	LEU D 151	101.760	58.396	21.227	1.00 16.50	D
ATOM	4176	CB	LEU D 151	102.849	58.705	20.203	1.00 15.48	D
ATOM	4177	CG	LEU D 151	103.806	59.825	20.639	1.00 17.55	D
ATOM	4178	CD1	LEU D 151	104.641	59.374	21.834	1.00 16.60	Ð
ATOM	4179	CD2		104.702	60.213	19.476	1.00 16.11	D
ATOM	4180	C	LEU D 151	101.140	59.701	21.693	1.00 17.56	D
				100.577	60.440	20.888	1.00 17.18	D
MOTA	4181	0	LEU D 151				1.00 16.14	D
ATOM	4182	N	THR D 152	101.233	59.997	22.983		
ATOM	4183	CA	THR D 152	100.690	61.259	23.448	1.00 19.47	D
MOTA	4184	CB	THR D 152	100.359	61.248	24.966	1.00 21.24	D
ATOM	4185	OG1	THR D 152	101.517	60.871	25.725	1.00 25.03	D
ATOM	4186	CG2	THR D 152	99.214	60.281	25.247	1.00 20.79	D
ATOM	4187	C	THR D 152	101.717	62.345	23.151	1.00 19.82	D
		0	THR D 152	102.921	62.113	23.218	1.00 21.31	D
MOTA	4188	_		101.241	63.523	22.781	1.00 20.76	D
MOTA	4189	N	LEU D 153				1.00 24.15	D
MOTA	4190	CA	LEU D 153	102.143	64.617	22.488		
MOTA	4191	CB	LEU D 153	102.760	64.450	21.089	1.00 25.45	Ď
MOTA	4192	CG	LEU D 153	101.959	64.575	19.785	1.00 27.17	D
MOTA	4193	CD1	LEU D 153	100.520	64.101	19.986	1.00 27.83	D
ATOM	4194	CD2	LEU D 153	101.982	66.015	19.319	1.00 27.38	D
	4195	C	LEU D 153	101.440	65.952	22.601	1.00 25.73	D
MOTA				100,208	66.028	22.681	1.00 26.55	D
MOTA	4196	0	LEU D 153				1.00 26.77	D
ATOM	4197	N	LEU D 154	102.251	67.000	22.640		
MOTA	4198	CA	LEU D 154	101.781	68.369	22.734	1.00 26.34	D
MOTA	4199	CB	LEU D 154	102.298	69.027	24.019	1.00 25.08	D
MOTA	4200	CG	LEU D 154	101.877	70.478	24.288	1.00 26.28	D
ATOM	4201	CD1	LEU D 154	100.377	70.531	24.570	1.00 24.44	D
ATOM	4202	CD2		102.667	71.031	25.477	1.00 23.08	D
ATOM	4202	C	LEU D 154	102.374			1.00 28.41	D
		_	LEU D 154	102.574			1.00 27.19	D
ATOM	4204	0					1.00 27.13	D
MOTA	4205	N	PRO D 155	101.534		20.523		
MOTA	4206	CD	PRO D 155	100.109	68.979	20.453	1.00 30.25	D
MOTA	4207	CA	PRO D 155	101.965	70.014		1.00 31.71	D
MOTA	4208	CB	PRO D 155	100.667	70.160	18.510	1.00 31.92	D
ATOM	4209	CG	PRO D 155	99.861	68.968	18.963	1.00 31.51	D
ATOM	4210	C	PRO D 155	102.663	71.354	19.508	1.00 35.12	D
ATOM	4211	-	PRO D 155	102.110			1.00 35.64	D
			SER D 156	103.893	71.436		1.00 39.00	D
ATOM	4212	N					1.00 42.94	D
MOTA	4213	CA	SER D 156	104.706	14.043	J. 7. UOJ	T.00 TZ.7T	مدة
					,	20		

ATOM	4214	CB	SER D	156	105.819	72.492	20.121	1.00 43.03	D
ATOM	4215	OG	SER D	156	105.288	72.385	21.430	1.00 45.30	D
ATOM	4216	C	SER D	156	105.311	72.763	17.694	1.00 46.03	D
MOTA	4217	0	SER D	156	104.875	72.084	16.770	1.00 47.06	D
MOTA	4218	N	ALA D	157	106.316	73.609	17.534	1.00 49.61	D _
ATOM	4219	CA	ALA D	157	106.931	73.756	16.222	1.00 51.03	D
ATOM	4220	CB	ALA D	157	106.977	75.231	15.828	1.00 51.20	D
ATOM	4221	C	ALA D	157	108.334 108.985	73.163 73.147	16.195 15.150	1.00 51.50 1.00 52.20	D D
ATOM	4222	O N	ALA D GLU D	157 158	108.797	72.669	17.339	1.00 52.20	D
ATOM ATOM	4223 4224	N CA	GLU D	158	110.141	72.103	17.411	1.00 53.43	D
ATOM	4224	CB	GLU D	158	110.946	72.785	18.524	1.00 57.17	D
MOTA	4225	CG	GLU D	158	110.401	72.570	19.934	1.00 61.50	D
ATOM	4227	CD	GLU D	158	109.278	73.529	20.291	1.00 63.75	D
ATOM	4228	OE1	GLU D	158	108.757	73.431	21.425	1.00 63.56	D
ATOM	4229	OE2	GLU D	158	108.922	74.381	19.445	1.00 65.17	D
ATOM	4230	C	GLU D	158	110.190	70.592	17.614	1.00 51.03	D
ATOM	4231	0	GLU D	158	111.103	70.084	18.265	1.00 51.07	D
ATOM	4232	N	GLU D	159	109.219	69.876	17.057	1.00 47.47	D
ATOM	4233	CA	GLU D	159	109.185	68.425	17.193	1.00 46.22	D
ATOM	4234	CB	GLU D	159	108.337	68.013	18.406	1.00 47.11	D
MOTA	4235	CG	GLU D	159	109.127	67.692	19.671	1.00 48.53	D
MOTA	4236	CD	GLU D	159	108.268	67.042	20.751	1.00 50.37	D
ATOM	4237	OE1	GLU D		107.319	67.694	21.238	1.00 50.39	D
ATOM	4238	OE2	GLU D		108.537	65.873	21.112 15.960	1.00 50.03 1.00 43.84	D D
ATOM	4239	C	GLU D		108.641 107.515	67.714 67.974	15.535	1.00 43.84	D
ATOM	4240	O N	GLU D SER D		107.515	66.825	15.380	1.00 39.56	D
ATOM ATOM	4241 4242	N CA	SER D		108.993	66.054	14.229	1.00 37.29	D
ATOM	4242	CB	SER D		109.971	66.172	13.055	1.00 37.41	D
ATOM	4244	OG	SER D		111.070	65.298	13.206	1.00 41.72	D
ATOM	4245	C	SER D		108.933	64.615	14.734	1.00 35.08	D
ATOM	4246	0	SER D		109.754	64.207	15.557	1.00 33.66	D
MOTA	4247	N	TYR D		107.961	63.846	14.260	1.00 32.11	D
ATOM	4248	CA	TYR D	161	107.828	62.478	14.728	1.00 29.69	D
ATOM	4249	CB	TYR D	161	106.550	62.315	15.547	1.00 29.62	D
MOTA	4250	CG	TYR D	161	106.347	63.349	16.620	1.00 29.33	D
MOTA	4251	CD1	TYR D	161	105.761	64.577	16.327	1.00 31.31	D -
MOTA	4252	CE1			105.513	65.515	17.329	1.00 32.70	D
ATOM	4253	CD2			106.695	63.085	17.937	1.00 30.13	D
ATOM	4254	CE2				64.013	18.947	1.00 30.43 1.00 31.92	D D
ATOM	4255	CZ	TYR D		105.863 105.592	65.223 66.128	18.638 19.643	1.00 31.92	D
ATOM	4256	OH C	TYR D		105.552	61.441	13.627	1.00 29.60	D
ATOM ATOM	4257 4258	0	TYR D		107.493	61.728	12.473	1.00 29.45	D
ATOM	4259	N	ASP D		108.172	60.221	14.005	1.00 29.35	D
ATOM	4260	CA	ASP D		108.201	59.109	13.075	1.00 30.15	D
ATOM	4261	CB	ASP D		109.618	58.863	12.548	1.00 34.90	D
ATOM	4262	CG	ASP D		110.154	60.016	11.733	1.00 37.70	D
MOTA	4263	OD1	ASP D	162	109.669	60.218	10.597	1.00 40.13	D
MOTA	4264	OD2	ASP D	162	111.061	60.716	12.235	1.00 38.68	D
ATOM	4265	C	ASP D	162	107.759	57.851	13.784	1.00 29.84	D
MOTA	4266	0		162	108.010	57.672	14.978	1.00 26.72	D
ATOM	4267	N	CYS I		107.088	56.984	13.039	1.00 29.31	D
MOTA	4268	CA	CYS I		106.684	55.700	13.569	1.00 29.59 1.00 28.04	D
ATOM	4269	C	CYS I		107.689	54.769	12.902 11.685	1.00 26.22	D D
ATOM	4270	O	CYS I		107.822 105.265	54.772 55.326	13.134	1.00 20.22	D
MOTA	4271 4272	CB SG	CYS I		103.203	53.760	13.878	1.00 34.32	D
ATOM ATOM	4272	N	LYS I		108.417	54.001	13.699	1.00 29.03	D
ATOM	4274	CA	LYS I		109.404	53.072	13.161	1.00 29.67	D
ATOM	4275	CB	LYS I		110.730	53.238	13.911	1.00 32.54	D
ATOM	4276	CG	LYS I		111.874	52.352	13.416	1.00 34.76	D
ATOM	4277	CD	LYS I	164	113.109	52.528	14.297	1.00 34.79	D
ATOM	4278	CE	LYS I	164	114.254	51.630	13.850	1.00 38.29	D
ATOM	4279	NZ	LYS I	164	115.425	51.702	14.775	1.00 36.58	D
MOTA	4280	C	LYS I		108.863	51.651	13.322	1.00 28.94	D
ATOM	4281	0	LYS I		108.642	51.189	14.443	1.00 29.32	D
MOTA	4282	N	VAL I		108.632	50.974	12.197	1.00 27.33	D
ATOM	4283	CA	VAL I		108.100	49.618	12.212	1.00 26.58	D
ATOM	4284	CB	VAL I		106.797	49.516	11.359 11.462	1.00 27.12 1.00 25.56	D D
MOTA	4285	CG1 CG2			106.199 105.787	48.122 50.544	11.402	1.00 25.56	D
MOTA MOTA	4286 4287	CGZ	VAL I		109.113	48.600	11.690	1.00 26.91	D
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ATOM	4288	0	VAL D 1	L65	109.621	48.720	10.583	1.00 25.56	D
ATOM	4289	N	Gra D	L66	109.414	47.606	12.513	1.00 28.75	D
ATOM	4290	CA		166	110.338	46.544	12.139	1.00 30.67	D
ATOM	4291	CB		L66	111.445	46.410	13.194	1.00 33.57	D D
ATOM	4292	CG		L66	112.452	47.565 47.526	13.142 14.244	1.00 41.68 1.00 46.12	D D
ATOM	4293	CD		166 166	113.506 114.482	48.304	14.146	1.00 49.01	D
ATOM ATOM	4294 4295	OE1 OE2		166	113.363	46.736	15.206	1.00 49.40	D
ATOM	4296	C		1.66	109.543	45.243	12.008	1.00 30.18	D
ATOM	4297	0		166	108.737	44.900	12.878	1.00 28.51	D
ATOM	4298	N		167	109.759	44.535	10.907	1.00 29.48	D
ATOM	4299	CA	HIS D	167	109.056	43.281	10.648	1.00 30.29	D
ATOM	4300	CB	HIS D	167	107.686	43.569	10.025	1.00 29.56	D
ATOM	4301	CG		167	106.808	42.363	9.903	1.00 30.02	D
ATOM	4302	CD2		167	106.562	41.541	8.856	1.00 29.91 1.00 31.27	D D
ATOM	4303	ND1		167 167	106.068 105.404	41.871 40.798	10.957 10.564	1.00 31.27	D
MOTA MOTA	4304 4305	CE1 NE2		167 167	105.404	40.736	9.293	1.00 28.97	D
ATOM	4305	C		167	109.886	42.440	9.684	1.00 30.36	D
ATOM	4307	0		167	110.607	42.976	8.842	1.00 30.66	D
ATOM	4308	N		168	109.775	41.122	9.801	1.00 31.13	D
ATOM	4309	CA	TRP D	168	110.521	40.219	8.930	1.00 32.08	D
ATOM	4310	CB	TRP D	168	110.270	38.765	9.336	1.00 28.28	D
ATOM	4311	CG		168	110.665	38.475	10.739	1.00 26.36	D
MOTA	4312	CD2		168	110.031	37.556	11.635 12.842	1.00 25.51 1.00 26.35	D D
MOTA	4313	CE2		168 168	110.759 108.916	37.578 36.715	11.534	1.00 24.88	D
ATOM ATOM	4314 4315	CE3		168	111.721	39.004	11.416	1.00 27.27	D
ATOM	4316	NE1		168	111.786	38.471	12.682	1.00 28.25	D
ATOM	4317	CZ2		168	110.412	36.791	13.943	1.00 27.00	D
ATOM	4318	CZ3	TRP D	168	108.568	35.932	12.628	1.00 25.90	D
MOTA	4319	CH2	TRP D	168	109.315	35.976	13.817	1.00 26.65	D -
ATOM	4320	C	TRP D	168	110.180	40.403	7.452	1.00 33.22	D
MOTA	4321	0		168	111.011	40.139	6.582	1.00 33.90	D
ATOM	4322	N	GLY D		108.959	40.853	7.174	1.00 34.75 1.00 36.14	D D
ATOM	4323	CA		169	108.533 109.056	41.060 42.359	5.797 5.215	1.00 37.80	D
ATOM	4324	C	GLY D	169	109.038	42.796	4.139	1.00 37.00	D
ATOM ATOM	4325 4326	N O	LEU D		109.979		5.938	1.00 38.89	D
ATOM	4327	CA	LEU D		110.578	44.234	5.509	1.00 40.79	D
ATOM	4328	CB	LEU D		110.212	45.356	6.480	1.00 39.77	D
ATOM	4329	CG	LEU D	170	108.745	45.765	6.581	1.00 39.57	D
ATOM	4330	CD1	LEU D	170	108.592	46.809	7.671	1.00 38.10	D
MOTA	4331	CD2		170	108.267	46.308	5.243	1.00 39.58	D
ATOM	4332	C	LEU D		112.092	44.085	5.465 6.370	1.00 42.12 1.00 41.54	D D
ATOM	4333	0	LEU D		112.688 112.706	43.506 44.613	4.411	1.00 45.36	D
ATOM	4334	N CA	ASP D ASP D		114.158	44.559	4.252	1.00 48.35	D
MOTA MOTA	4335 4336	CB	ASP D		114.539	44.947	2.820	1.00 50.69	D
ATOM	4337	CG	ASP D		113.467	45.775	2.137	1.00 52.75	D
ATOM	4338		ASP D		113.076	46.827	2.689	1.00 54.19	D
ATOM	4339	OD2	ASP D	171	113.012	45.372	1.046	1.00 54.32	D
ATOM	4340	C	ASP D	171	114.849	45.485	5.255	1.00 48.43	D
MOTA	4341	0	ASP D		115.816	45.090	5.910	1.00 48.29	D
MOTA	4342	N	LYS D		114.348	46.715	5.364	1.00 48.92 1.00 49.86	D
MOTA	4343	CA	LYS D		114.883	47.707	6.299 5.552	1.00 49.88	D D
MOTA	4344	CB	LYS D		115.502 116.667	48.898 48.566	4.637	1.00 55.86	D
ATOM	4345 4346	CG CD	LYS D		116.203	47.963		1.00 58.23	D
ATOM ATOM	4347	CE	LYS D		115.408	48.966	2.493	1.00 59.62	D
ATOM	4348	NZ	LYS D		114.946	48.368	1.211	1.00 59.53	D
ATOM	4349	C	LYS D		113.734	48.224	7.165	1.00 48.46	D
ATOM	4350	0	LYS D	172	112.564	48.026		1.00 48.43	D
ATOM	4351	N	PRO D	173	114.050	48.885	8.291	1.00 46.54	D
ATOM	4352	CD	PRO D		115.355	49.048			D
ATOM	4353	CA	PRO D		112.974	49.400			D D
MOTA	4354	CB	PRO D		113.722	50.029 49.197		1.00 44.19	D D
MOTA	4355 4356	CG C	PRO D		114.950 112.180	50.430		1.00 43.26	D
ATOM ATOM	4356 4357	0	PRO D		112.746	51.197		1.00 43.42	D
ATOM	4358	N	LEU D		110.869	50.434		1.00 41.53	D
MOTA	4359		LEU D		110.023	51.381		1.00 39.96	D
ATOM	4360		LEU D		108.675	50.730		1.00 40.30	D
MOTA	4361	CG	LEU D	174	107.900	51.223	6.303	1.00 40.55	D

ATOM	4362	CD1	LEU	D	174	10	06.637	5	50.397	6	.151	1.0	00	42.25	D
ATOM	4363	CD2	LEU	D	174	10	7.568		52.698	6	.448	1.0	00	42.67	D
ATOM	4364	С	LEU	D	174	10	9.845		52.586	8	.753	1.0	00	39.80	D
ATOM	4365	0	LEU		174	10	9.645		52.420	9	.955	1.0	00	39.99	D
ATOM	4366	N		D	175	10	9.947	<u> </u>	53.792	8	3.200	1.	00	38.49	D
ATOM	4367	CA		D	175		09.787		55.016		.983	1.0			D
ATOM	4368	CB		D	175		11.095		55.812		.045			38.62	D
ATOM	4369	CG	LEU		175		12.127		55.442		1113	1.			Đ
			LEU		175		11.518		55.648		489			39.24	D
ATOM	4370	CD1										1.0			D
ATOM	4371	CD2	LEU		175		12.577		54.001		9.936				
ATOM	4372	C	LEU		175		08.712		55.892		3.372			37.31	D
ATOM	4373	0	LEU		175		08.885		56.432		7.282	1.			D
ATOM	4374	N	LYS		176		07.599		56.033		0.076			35.14	D
ATOM	4375	CA	LYS		176		06.511		56.850		3.577	1.			
MOTA	4376	CB	LYS	D	176	10	05.175		56.124		3.768			33.88	D
MOTA	4377	CG	LYS	D	176	10	04.204	: !	56.325	7	7.620	1.	00	36.72	D
ATOM	4378	CD	LYS	D	176	10	04.829	!	55.887	e	5.295	1.	00	37.68	D
MOTA	4379	CE	LYS	D	176	10	03.820) !	55.913	5	5.155	1.	00	39.32	D
MOTA	4380	NZ	LYS	D	176	10	03.195	; !	57.254	4	1.974	1.	00	40.75	D
ATOM	4381	C	LYS	D	176	10	06.523	, ,	58.166	9	3.335	1.	00	32.22	D
ATOM	4382	0	LYS	D	176	10	06.272		58.204	10	.537	1.	00	32.35	D
ATOM	4383	N	HIS	D	177	10	06.825	; !	59.243	8	3.625	1.	00	29.85	D
ATOM	4384	CA	HIS	D	177	10	06.897	, (60.563	ç	229	1.	00	29.87	D
ATOM	4385	CB			177		07.836		61.456		3.411	1.	00	30.84	D
ATOM	4386	CG	HIS				08.014		62.830		3.979			31.41	D
ATOM	4387	CD2		D	177		07.607		64.042		3.529			32.01	D
	4388	ND1		D	177		08.695		63.067		0.155	1.			D
ATOM			HIS	D	177		08.704		64.365		0.402	1.			D
ATOM	4389	CE1			177		08.70 1 08.051		64.979		9.431	1.			D
ATOM	4390	NE2		D			05.532		61.228		9.332	1.			
ATOM	4391	C	•	D	177		03.33 <i>2</i> 04.709		61.121		3.429	1.			
ATOM	4392	0		D	177				61.922		0.439	1.			D
ATOM	4393	N	TRP	D	178		05.295		62.617		0.619	1.			D
ATOM	4394	CA	TRP	D	178		04.031				2.048	1.			D
ATOM	4395	CB	TRP	D	178		03.518		62.464		2.243	1.			
ATOM	4396	CG	TRP	D	178		02.205		63.165						
MOTA	4397	CD2		D	178		01.939		64.262		3.122	1.			
ATOM	4398	CE2	TRP	D	178		00.580		64.608		2.959	1.			
ATOM	4399	CE3		D	178		02.714		64.986		4.033				
ATOM	4400	CD1		D	178		01.028		62.898		1.599		00		
MOTA	4401	NE1		D	178		00.050		63.759		2.023	1.			
MOTA	4402	CZ2		D			99.980		65.649		3.675		00		
MOTA	4403	CZ3	TRP	D			02.118		66.021		4.746			27.98	
MOTA	4404	CH2	TRP	D			00.763		66.340		4.562			27.02	
MOTA	4405	C	TRP	D			04.185		64.100		0.294			30.33	
ATOM	4406	0	TRP	D			04.756		64.824		1.143		00		
ATOM	4407	OXT	TRP	D	178		03.745		64.512		9.193		00		
MOTA	4408	CB	SER	E	3		13.641		35.776		8.019		00		
MOTA	4409	OG	SER	E	3	1.	12.349		35.748		8.608			59.65	
ATOM	4410	C	SER	E	3	1	14.352	2	33.977		9.601		00		
ATOM	4411	0	SER	E	3	1	14.571		32.945		8.970			57.45	
ATOM	4412	N	SER	\mathbf{E}	3		16.055		35.305		8.352			59.31	
ATOM	4413	CA	SER	E	3	1	14.719	€	35.342	-	9.020			58.85	
MOTA	4414	N	PRO	E	4	1	13.799	€	33.958	1	0.824		00		
ATOM	4415	CD	PRO	E	4	1	13.679	€	35.092	1:	1.759	1.	00	56.20	
ATOM	4416	CA	PRO	E	4	1	13.403	3	32.704	1.	1.472	1.	00	55.50	
ATOM	4417	CB	PRO	E	4	1	13.362	2	33.086	1:	2.946	1.	00	56.49	E
ATOM	4418	CG	PRO	E	4	1	12.870	3	34.493	1.	2.893	1.	00	56.56	E
ATOM	4419	С	PRO	E	4	1	12.046	5	32.217	1	0.957	1.	00	53.68	E
ATOM	4420	0	PRO	E	4	1	11.168	В	33.024	1	0.648	1.	00	54.06	E
ATOM	4421	N	GLU	E	5	1	11.875	5	30.903	1	0.855	1.	00	51.52	E
MOTA	4422	CA	GLU	E	5	1	10.610	0	30.360	1	0.373	1.	00	49.69	E
MOTA	4423	СВ	GĽU			1	10.831	1.	29.007		9.676	1.	0.0	53.42	E
ATOM	4424	CG	GLU			1	11.305	5	27.867	1	0.561	1.	00	57.99	E
MOTA	4425	CD	GLU			1	11.671	1	26.626		9.758	1.	00	60.86	E
ATOM	4426	OE1					10.857		26.196		8.908			62.41	
ATOM	4427	OE2					12.772		26.077		9.979	1.	00	63.42	E
ATOM	4428	C	GLU				.09.619		30.231		1.525	1.	00	45.48	E
ATOM	4429	0	GLU				.09.919		29.644		2.564	1.	00	46.07	E
ATOM	4430	N	ASP				.08.436		30.800	1	1.337	1.	00	40.87	E
ATOM	4431	CA	ASP				07.403		30.782		2.363			36.20	
ATOM	4432	CB	ASP				.06.911		32.214		2.617			35.53	
ATOM	4433	CG	ASP				.05.995		32.323		3.827			33.60	
ATOM	4434		ASP				.05.185		33.268		3.864			34.88	
ATOM	4435		ASP				.06.089		31.487		4.748		. 00	33.84	E E
	_		- -												

ATOM	4436	C	ASP	E	6	106.229	29.915	11.938	1.00 33.07	${f E}$
ATOM	4437	0	ASP	E	6	105.882	29.867	10.762	1.00 32.95	E
ATOM	4438	N		E	7	105.632	29.228	12.906	1.00 31.08	E
		CA		E	7	104.466	28.380	12.669	1.00 29.18	E
ATOM	4439							13.116	1.00 31.11	E
ATOM	4440	CB	PHE	E	7	104.760	26.950			
MOTA	4441	CG	PHE	E	7	105.833	26.278	12.305	1.00 31.97	E
ATOM	4442	CD1	PHE	\mathbf{E}	7	105.544	25.745	11.053	1.00 31.67	E
ATOM	4443	CD2	PHE	E	7	107.141	26.200	12.782	1.00 32.49	E
ATOM	4444	CE1	PHE	E	7	106.546	25.141	10.282	1.00 33.41	E
ATOM	4445	CE2	PHE	E	7	108.148	25.602	12.023	1.00 32.29	E
						107.850	25.071	10.770	1.00 31.62	E
ATOM	4446	CZ	PHE	E	7					
ATOM	4447	C	PHE	E	7	103.345	28.994	13.504	1.00 27.19	E
MOTA	4448	0	PHE	E	7	103.483	29.151	14.715	1.00 25.77	E
MOTA	4449	N	VAL	E	8	102.238	29.340	12.855	1.00 25.52	E
ATOM	4450	CA	VAL	E	8	101.127	29.998	13.538	1.00 23.97	E
ATOM	4451	CB	VAL	E	8	100.903	31.411	12.949	1.00 22.51	E
ATOM	4452	CG1		E	8	99.789	32.130	13.703	1.00 20.58	E
						102.205	32.211	13.002	1.00 22.51	E
ATOM	4453	CG2		E	8					
MOTA	4454	C		E	8	99.785	29.275	13.510	1.00 24.21	E
ATOM	4455	0	VAL	E	8	99.369	28.736	12.485	1.00 25.26	E
ATOM	4456	N	TYR	E	9 '	99.096	29.288	14.643	1.00 23.98	E
MOTA	4457	CA	TYR	\mathbf{E}	9	97.786	28.663	14.724	1.00 23.53	E
ATOM	4458	CB	TYR	E	9	97.796	27.505	15.718	1.00 24.07	E
ATOM	4459	CG	TYR		9	96.562	26.640	15.627	1.00 25.27	E
							25.460	14.889	1.00 27.68	E
ATOM	4460	CD1	TYR		9	96.570				E
MOTA	4461	CE1	TYR		9	95.435	24.658	14.801	1.00 27.67	
MOTA	4462	CD2	TYR	E	9	95.384	27.002	16.272	1.00 24.82	E
MOTA	4463	CE2	TYR	\mathbf{E}	9	94.245	26.211	16.191	1.00 25.29	E
ATOM	4464	CZ	TYR	E	9	94.277	25.040	15.458	1.00 26.82	E
ATOM	4465	OH	TYR	E	9	93.163	24.240	15.403	1.00 27.65	${f E}$
ATOM	4466	C	TYR		9	96.775	29.707	15.179	1.00 23.14	E
	4467	0	TYR		9	97.037	30.476	16.106	1.00 23.66	E
MOTA								14.523	1.00 21.64	E
MOTA	4468	N	GLN		10	95.622	29.739			
ATOM	4469	CA	GLN	E	10	94.582	30.686	14.892	1.00 21.14	E
ATOM	4470	CB	GLN	\mathbf{E}	10	94.438	31.793	13.843	1.00 20.35	E
ATOM	4471	CG	GLN	\mathbf{E}	10	95.677	32.598	13.529	1.00 19.58	E
ATOM	4472	CD	GLN	E	10	95.410	33.655	12.461	1.00 18.44	E
ATOM	4473	OE1	GLN	E	10	94.498	34.474	12.593	1.00 19.00	${f E}$
ATOM	4474	NE2	GLN		10	96.206	33.640	11.400	1.00 18.89	E
						93.232	29.997	15.006	1.00 19.74	E
ATOM	4475	C	GLN		10					E
MOTA	4476	0	-		10	92.904	29.113	14.223	1.00 21.71	
ATOM	4477	N	PHE	E	11	92.450	30.408	15.991	1.00 19.13	E
ATOM	4478	CA	PHE	\mathbf{E}	11	91.108	29.887	16.145	1.00 16.86	E
ATOM	4479	CB	PHE	E	11	90.981	28.881	17.271	1.00 16.74	E
ATOM	4480	CG	PHE	E	11	89.562	28.466	17.517	1.00 18.71	E
MOTA	4481	CD1	PHE	E	11	88.910	27.615	16.626	1.00 21.10	E
ATOM	4482	CD2			11	88.849	28.985	18.595	1.00 18.11	E
						87.559	27.290	16.807	1.00 22.40	E
MOTA	4483	CE1			11					
MOTA	4484	CE2	PHE	E	11	87.499	28.671	18.789	1.00 15.75	E
ATOM	4485	CZ	PHE	E	11	86.854	27.826	17.898	1.00 21.25	E
MOTA	4486	C	PHE	E	11	90.218	31.069	16.451	1.00 17.10	E
ATOM	4487	0	PHE	E	11	90.461	31.819	17.406	1.00 13.97	${f E}$
ATOM	4488	N	LYS		12	89.197	31.241	15.622	1.00 16.07	E
ATOM	4489	CA	LYS		12	88.266	32.338	15.789	1.00 16.96	E
						88.308	33.246	14.564	1.00 17.05	E
MOTA	4490	CB	LYS		12					E
MOTA	4491	CG	LYS		12	89.703	33.748	14.200	1.00 17.57	
MOTA	4492	CD	LYS	E	12	89.663	34.535	12.888	1.00 18.92	E
ATOM	4493	CE	LYS	E	12	91.018	35.136	12.532	1.00 17.07	E
MOTA	4494	NZ	LYS	E	12	90.920	36.063	11.362	1.00 14.26	${f E}$
ATOM	4495	C	LYS	E	12	86.856	31.803	15.987	1.00 17.87	· E
ATOM	4496	Ō	LYS		12	86.354	31.039	15.165	1.00 16.82	E
						86.235	32.195	17.098	1.00 18.19	E
MOTA	4497	N	GLY		13				1.00 19.62	E
ATOM	4498	CA	GLY		13	84.875	31.776	17.391		
MOTA	4499	C	GLY		13	83.991	32.939	17.010	1.00 19.93	E
ATOM	4500	0	GLY	E	13	83.539	33.695	17.868	1.00 21.65	E
ATOM	4501	N	MET	E	14	83.728	33.070	15.715	1.00 19.89	E
ATOM	4502	CA	MET		14	82.947	34.184	15.197	1.00 20.54	E
ATOM	4503	CB	MET		14	83.430	34.490	13.785	1.00 21.02	E
MOTA	4504	CG	MET		14	84.937	34.657	13.751	1.00 23.04	E
						85.587	35.218	12.190	1.00 25.32	E
ATOM	4505	SD	MET		14					E
ATOM	4506	CE	MET		14	85.218	36.938	12.284	1.00 20.32	
MOTA	4507	C	MET		14	81.429	34.078	15.219	1.00 20.83	E
ATOM	4508	0	MET	E	14	80.859	32.999	15.101	1.00 20.77	E
MOTA	4509	N	CYS	E	15	80.789	35.232	15.377	1.00 20.66	E

MOTA	4510	CA	CYS	E	15	79.332	35.336	15.418	1.00 22.09	E
ATOM	4511	С	CYS	E	15	78.882	36.495	14.524	1.00 21.39	E
ATOM	4512	0	CYS	E	15	79.393	37.614	14.644	1.00 19.38	E
ATOM	4513	CB		E	15	78.841	35.616	16.848	1.00 22.10	E
ATOM	4514	SG		E	15	78.970	34.281	18.094	1.00 26.75	E
ATOM	4515	N	TYR		16	77.931	36.229	13.633	1.00 20.94	E
ATOM	4516	CA	TYR		16	77.408	37.270	12.752	1.00 21.23	E
ATOM	4517	CB	TYR		16	77.548	36.858	11.287	1.00 18.37	E
	4518	CG	TYR		16	78.972	36.574	10.876	1.00 19.23	E
ATOM		CD1	TYR		16	79.576	35.354	11.178	1.00 18.71	· E
ATOM	4519					80.875	35.084	10.789	1.00 18.69	E
ATOM	4520	CE1	TYR		16		37.524	10.733	1.00 20.25	E
ATOM	4521	CD2	TYR		16	79.715	37.324	9.785	1.00 20.25	E
ATOM	4522	CE2	TYR		16	81.022	36.047	10.088	1.00 21.03	E
ATOM	4523	CZ	TYR		16	81.595			1.00 21.03	E
ATOM	4524	OH	TYR		16	82.872	35.775	9.662		E
ATOM	4525	C	TYR		16	75.938	37.543	13.085		E
ATOM	4526	0	TYR		16	75.132	36.612	13.199	1.00 21.71	
ATOM	4527	N	PHE	E	17	75.607	38.825	13.247	1.00 23.05	E
ATOM	4528	CA	PHE	E	17	74.254	39.263	13.591	1.00 23.67	E
ATOM	4529	CB	PHE	E	17	74.261	39.988	14.942	1.00 22.49	E
ATOM	4530	CG	PHE	E	17	74.813	39.172	16.084	1.00 25.10	E
ATOM	4531	CD1	PHE	E	17	74.007	38.270	16.772	1.00 24.22	E
ATOM	4532	CD2	PHE	E	17	76.140	39.318	16.482	1.00 24.67	E
MOTA	4533	CE1	PHE	E	17	74.516	37.526	17.844	1.00 24.68	E
MOTA	4534	CE2	PHE	E	17	76.656	38.579	17.548	1.00 24.45	E
MOTA	4535	CZ	PHE	E	17	75.843	37.684	18.228	1.00 24.13	E
MOTA	4536	C	PHE	E	17	73.673	40.223	12.549	1.00 25.10	E
MOTA	4537	0	PHE	E	17	74.390	41.034	11.971	1.00 24.65	E
ATOM	4538	N	THR	E	18	72.365	40.122	12.333	1.00 27.15	E
ATOM	4539	CA	THR	E	18	71.638	40.983	11.405	1.00 29.69	E
ATOM	4540	CB	THR	\mathbf{E}	18	71.609	40.397	9.978	1.00 29.46	E
ATOM	4541	OG1	THR	E	18	72.949	40.252	9.500	1.00 32.31	E
ATOM	4542	CG2	THR	E	18	70.863	41.321	9.032	1.00 28.09	E
ATOM	4543	C	THR	E	18	70.217	41.080	11.950	1.00 31.56	E
MOTA	4544	0	THR	E	18	69.638	40.071	12.355	1.00 32.09	E
ATOM	4545	N	ASN	E	19	69.661	42.290	11.969	1.00 33.38	E
ATOM	4546	CA.	ASN	E	19	68.316	42.495	12.497	1.00 35.02	E
ATOM	4547	CB	ASN		19	67.279	41.755	11.647	1.00 37.99	E
ATOM	4548	CG	ASN		19	66.779	42.587	10.489	1.00 42.21	E
ATOM	4549	OD1	ASN		19	66.271	43.695	10.687	1.00 47.70	E
ATOM	4550	ND2			19	66.910	42.063	9.273	1.00 43.13	E
ATOM	4551	C	ASN		19	68.264	41.977	13.924	1.00 34.10	E
ATOM	4552	0	ASN		19	67.487	41.077	14.233	1.00 34.27	E
ATOM	4553	N	GLY		20	69.088	42.553	14.795	1.00 33.50	E
ATOM	4554	CA	GLY		20	69.120	42.106	16.175	1.00 33.61	E
ATOM	4555	C	GLY		20	69.575	40.663	16.175	1.00 33.98	E
ATOM	4556	0	GLY		20	70.580	40.343	15.541	1.00 34.56	E
	4557		THR		21	68.847	39.789	16.866	1.00 34.08	E
ATOM		N	THR		21	69.198	38.372	16.897	1.00 35.71	E
ATOM	4558	CA			21	69.193	37.809	18.335	1.00 37.69	E
ATOM	4559	CB	THR			67.907	38.026	18.930	1.00 37.33	E
ATOM	4560	OG1			21	70.268	38.480	19.174	1.00 38.05	E
ATOM	4561	CG2			21	68.251	37.517	16.050	1.00 35.19	E
ATOM	4562	C	THR		21	68.251	36.324	16.303	1.00 36.08	E
ATOM	4563	0	THR		21		38.129	15.052	1.00 34.15	E
MOTA	4564	И	GLU		22	67.619		14.176	1.00 34.13	E
ATOM	4565	CA	GLU		22	66.705	37.405		1.00 34.00	E
MOTA	4566	CB	GLU		22	65.868	38.388	13.354		E
MOTA	4567	CG	GLU		22	64.781	39.073	14.164	1.00 33.66	E
ATOM	4568	CD	GLU		22	64.173	40.266	13.451	1.00 35.85	E
ATOM	4569	OE1			22	63.865	40.151	12.244	1.00 35.10	E
MOTA	4570	OE2			22	63.995	41.317	14.105	1.00 38.34	
ATOM	4571	C	GLU	E	22	67.523	36.503	13.265	1.00 33.80	E
ATOM	4572	0	GLU	E	22	67.205	35.329	13.092	1.00 34.50	E
MOTA	4573	N	ARG	E	23	68.574	37.065	12.678	1.00 33.59	E
MOTA	4574	CA	ARG	E	23	69.467	36.298	11.818	1.00 33.75	E
ATOM	4575	CB	ARG	E	23	69.703	36.996	10.470	1.00 36.33	E
ATOM	4576	CG	ARG	E	23	68.599	36.815	9.434	1.00 42.06	E
MOTA	4577	CD	ARG	E	23	67.342	37.577	9.813	1.00 47.83	E
ATOM	4578	NE	ARG	E	23	66.408	37.696	8.695	1.00 51.02	E
ATOM	4579	CZ	ARG		23	65.349	38.502	8.690	1.00 52.66	E
ATOM	4580	NHI			23	65.087	39.263	9.747	1.00 50.82	E
MOTA	4581	NH2			23	64.555	38.555	7.626	1.00 53.53	E
ATOM	4582	C	ARG		23	70.788	36.177	12.560	1.00 30.98	E
MOTA	4583	0	ARG		23	71.465	37.172	12.827	1.00 30.90	E
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ATOM	4584	N	VAL	E	24	71.149 34.955 12.	909 1	L.00 28.33	E
ATOM	4585	CA	VAL		24	72.394 34.735 13.	621]	L.00 25.06	E
ATOM	4586	CB	VAL		24	72.148 34.500 15.	129	L.00 22.98	E
ATOM	4587	CG1	VAL		24	73.456 34.106 15.	817	1.00 21.05	E
ATOM	4588	CG2	VAL		24	71.582 35.762 15.	763	L.00 21.04	E
ATOM	4589	C	VAL		24		.049	1.00 23.08	E
ATOM	4590	0	VAL		24		.914	1.00 24.17	E
ATOM	4591	N	ARG		25			1.00 23.02	E
	4592	CA	ARG		25	• • • • • •		1.00 23.30	E
ATOM			ARG		25			1.00 24.06	E
ATOM	4593	CB			25	, = - =		1.00 25.99	E
ATOM	4594	CG	ARG			, , , , , , , , , , , , , , , , , , , ,		1.00 28.29	E
ATOM	4595	CD	ARG		25			1.00 29.69	E
ATOM	4596	NE	ARG		25	_		1.00 29.57	E
ATOM	4597	CZ	ARG		25	_	-	1.00 27.28	E
ATOM	4598	NH1	ARG		25				E
ATOM	4599	NH2	ARG		25			-	E E
ATOM	4600	C	ARG		25			1.00 22.65	
ATOM	4601	0	ARG	E	25			1.00 22.47	E
MOTA	4602	N	LEU	E	26		_	1.00 21.04	E
MOTA	4603	CA	LEU	E	26	, , , , , , , , , , , , , , , , , , , ,		1.00 21.94	E
MOTA	4604	CB	LEU	E	26			1.00 21.37	E
MOTA	4605	CG	LEU	E	26	·	-	1.00 22.89	E
MOTA	4606	CD1	LEU	E	26	78.723 29.567 17.	•	1.00 25.16	E
ATOM	4607	CD2	LEU	E	26	79.483 28.466 15	.493	1.00 23.51	E
ATOM	4608	С	LEU	\mathbf{E}	26	79.032 30.552 13	.193	1.00 21.17	E
ATOM	4609	0	LEU	E	26	78.637 29.674 12	.432	1.00 21.77	E
ATOM	4610	N	VAL	E	27	80.285 30.983 13	.201	1.00 19.92	${f E}$
ATOM	4611	CA	VAL		27	81.278 30.358 12	.345	1.00 21.31	E
ATOM	4612	CB	VAL		27	81.530 31.166 11	.039	1.00 20.44	E
ATOM	4613	CG1			27	82.524 30.420 10	.156	1.00 21.63	E
ATOM	4614	CG2			27		.275	1.00 20.48	E
MOTA	4615	C	VAL		27		.112	1.00 21.74	E
MOTA	4616	0	VAL		27			1.00 24.11	E
		N	SER		28			1.00 20.88	\mathbf{E}
ATOM	4617		SER		28	4 - 1 - - - - - - - - - -		1.00 21.53	E
ATOM	4618	CA			28	<u> </u>	_	1.00 20.62	E
MOTA	4619	CB	SER			••••		1.00 29.22	E
ATOM	4620	OG	SER		28			1.00 21.41	E
MOTA	4621	C	SER		28			1.00 19.11	E
MOTA	4622	0	SER		28	<u> </u>		1.00 18.23	E
MOTA	4623	N	ARG		29		.105	1.00 18.45	E
ATOM	4624	CA	ARG		29			1.00 16.45	E
ATOM	4625	CB	ARG		29				E
MOTA	4626	CG	ARG		29		.810	1.00 17.70	
ATOM	4627	$^{\mathrm{CD}}$	ARG	E	29		.109	1.00 18.98	E
ATOM	4628	NE	ARG	E	29		.705	1.00 20.82	E
ATOM	4629	CZ	ARG	E	29		.586	1.00 22.76	E
MOTA	4630	NH1	. ARG	E	29		.743	1.00 21.05	E
MOTA	4631	NH2	ARG	E	29		.309	1.00 20.13	E
ATOM	4632	C	ARG	E	29	88.842 28.435 12	.710	1.00 18.44	E
ATOM	4633	0	ARG	E	29	89.401 29.171 13	.520	1.00 19.35	E
ATOM	4634	N	SER	E	30	89.351 27.269 12	2.315	1.00 18.98	E
ATOM	4635	CA	SER	E	30	90.657 26.788 12	2.774	1.00 21.70	E
ATOM	4636	СВ	SEF	E S	30	90.619 25.284 13	.028	1.00 22.10	E
ATOM	4637	OG	SEF		30	89.718 24.969 14	1.072	1.00 27.24	${f E}$
ATOM	4638	C	SEF		30	91.637 27.119 11	639	1.00 23.03	\mathbf{E}
ATOM	4639	0	SEF		30	91.509 26.604 10	.528	1.00 23.56	E
ATOM	4640	N		EE	31		1.927	1.00 23.05	E
	4641	CA		EE	31	-).923	1.00 22.24	E
ATOM		CB		E	31		0.856	1.00 22.84	E
ATOM	4642				31	· · · · · · · · · · · · · · · · · ·	9.545	1.00 19.19	E
MOTA	4643	CG2		E	31	-	L.043	1.00 24.76	E
ATOM	4644	CG		E			0.047	1.00 29.25	E
MOTA	4645	CD:		E 5	31		1.134	1.00 24.53	E
ATOM	4646			E	31		2.225	1.00 24.33	E
ATOM	4647			EE		_	0.081	1.00 22.34	E
ATOM	4648			R E				1.00 24.41	E
MOTA	4649			RE	32		0.120	1.00 24.27	E
MOTA	4650			RE	32		9.417		E
MOTA	4651			RE			9.444	1.00 29.24	E
ATOM	4652			R E			0.649	1.00 30.69	E
MOTA	4653			R E			0.683	1.00 32.83	E
MOTA	4654			R E		-	8.267	1.00 31.46	E
MOTA	4655	CE		R E			8.288	1.00 32.58	
MOTA	4656	CZ	TY.	R E	32	—	9.497	1.00 32.80	E E
MOTA	4657	OH	TY	R E	32	102.768 24.280	9.522	1.00 33.44	Ti.
						00			

ATOM	4658	С	TYR	E	32	97.700	28.225	9.353	1.00 24.83	E
ATOM	4659	0	TYR	E	32	97.444	28.415	8.164	1.00 25.49	E
ATOM	4660	N	ASN	E	33	98.543	28.985	10.045	1.00 24.28	E
ATOM	4661	CA	ASN	\mathbf{E}	33	99.202	30.146	9.461	1.00 24.25	E
ATOM	4662	CB	ASN	E	33	100.144	29.740	8.324	1.00 23.93	E
MOTA	4663	CG	ASN	E	33	101.379	29.014	8.834	1.00 25.26	E
ATOM	4664	OD1		E	33	102.003	29.439	9.808	1.00 26.40	E
ATOM	4665	ND2	ASN	E	33	101.737	27.918	8.181	1.00 25.47	E
MOTA	4666	C	ASN		33	98.114	31.099	8.980	1.00 24.88	E
ATOM	4667	0	ASN		33	97.494	31.780	9.799	1.00 25.88	E
MOTA	4668	N	ARG		34	97.864	31.163	7.677	1.00 24.52	E
MOTA	4669	CA	ARG		34	96.815	32.055	7.194	1.00 26.32 1.00 26.61	E E
ATOM	4670	CB	ARG		34	97.385	33.175	6.317 7.072	1.00 26.81	E
ATOM	4671	CG	ARG		34	97.999 97.776	34.346 35.646	6.304	1.00 28.18	E
ATOM	4672	CD	ARG ARG		34 34	97.76	35.429	4.865	1.00 31.86	E
ATOM	4673 4674	NE CZ	ARG		34	97.607	36.332	3.931	1.00 33.42	E
ATOM ATOM	4675	NH1	ARG		34	97.197	37.550	4.265	1.00 35.40	E
ATOM	4676	NH2	ARG		34	97.722	36.003	2.653	1.00 35.29	E
ATOM	4677	C	ARG		34	95.728	31.333	6.417	1.00 26.98	E
ATOM	4678	0	ARG		34	94.896	31.968	5.763	1.00 28.88	E
ATOM	4679	N	GLU		35	95.719	30.010	6.481	1.00 26.13	E
ATOM	4680	CA	GLU		35	94.698	29.279	5.759	1.00 27.02	E
ATOM	4681	CB	GLU	E	35	95.350	28.359	4.720	1.00 31.96	E
MOTA	4682	ÇG	GLU	E	35	96.284	27.301	5.278	1.00 38.52	玉
ATOM	4683	CD	GLU	\mathbf{E}	35	97.116	26.633	4.192	1.00 42.24	E
MOTA	4684	OE1	GLU	E	35	98.180	27.187	3.832	1.00 44.86	E
MOTA	4685	OE2	GLU	E	35	96.699	25.565	3.690	1.00 43.70	E
MOTA	4686	C	GLU	E	35	93.754	28.498	6.671	1.00 25.31	E
ATOM	4687	0	GLU		35	94.175	27.709	7.522	1.00 22.18	E
MOTA	4688	N	GLU		36	92.464	28.756	6.498	1.00 24.46	E E
MOTA	4689	CA	GLU		36	91.438	28.085	7.272	1.00 24.13 1.00 24.37	E
MOTA	4690	CB	GLU		36	90.085	28.731	7.001 7.928	1.00 25.26	E
ATOM	4691	CG	GLU		36	88.975	28.295 28.991	7.604	1.00 25.20	E
ATOM	4692	CD	GLU		36 36	87.669 87.672	29.847	6.694	1.00 27.25	E
ATOM	4693	OE1			36 36	86.646	28.689	8.253	1.00 27.12	E
MOTA	4694 4695	OE2 C	GLU		36	91.413	26.630	6.826	1.00 23.40	E
ATOM ATOM	4695	0	GLU		36	91.252	26.347	5.645	1.00 23.72	E
ATOM	4697	И	ILE		37	91.576	25.707	7.767	1.00 23.97	E
ATOM	4698	CA	ILE		37	91.579	24.294	7.419	1.00 24.33	E
ATOM	4699	CB	ILE		37	92.818	23.578	8.019	1.00 24.98	E
ATOM	4700	CG2			37	94.096	24.255	7.532	1.00 24.26	E
MOTA	4701	CG1	ILE	E	37	92.771	23.616	9.544	1.00 25.10	E
ATOM	4702	CD3	ILE	E	37	93.822	22.742	10.204	1.00 26.49	E
ATOM	4703	C	ILE	E	37	90.301	23.555	7.836	1.00 23.49	E
ATOM	4704	0	ILE	EE	37	89.871	22.627	7.162	1.00 23.62	E
ATOM	4705	И	VAI	E	38	89.690	23.975	8.936	1.00 25.16	E
ATOM	4706	CA	IAV		38	88.465	23.342	9.415	1.00 25.85	E E
ATOM	4707	CB	VAI		38	88.715	22.489	10.667	1.00 26.44 1.00 27.10	E
MOTA	4708		L VAI		38	87.516	21.610	10.932 10.495	1.00 27.10	E
ATOM	4709	CG2			38	89.980	21.671 24.428	9.792	1.00 24.45	E
ATOM	4710	C	IAV		38 38	87.481 87.885	25.471	10.288	1.00 24.36	E
MOTA	4711	O N	VAI		39	86.193	24.168	9.594	1.00 24.90	E
MOTA MOTA	4712 4713	N CA	ARC		39	85.175	25.161	9.904	1.00 23.66	E
ATOM	4714	CB	ARC		39	84.975	26.055	8.678	1.00 25.55	E
ATOM	4715	CG	ARC		39	83.956	27.174	8.857	1.00 29.11	E
ATOM	4716	CD	ARO		39	83.514	27.755	7.515	1.00 29.37	E
ATOM	4717	NE		3 E	39	84.626	28.289	6.739	1.00 29.70	E
ATOM	4718	CZ	ARO	3 E		84.505	28.798	5.516	1.00 31.37	E
ATOM	4719	NH:	1 ARG	3 E	39	83.314	28.842	4.930	1.00 33.54	E
ATOM	4720	NH:	2 ARC	3 E	39	85.572	29.266	4.879	1.00 27.78	E
MOTA	4721	C	ARO	3 E	39	83.813	24.594	10.328	1.00 23.51	E
ATOM	4722	0	AR	З Е	39	83.385		9.853	1.00 23.83	E
MOTA	4723	N	PH	E E		83.147		11.242	1.00 22.04	E
MOTA	4724					81.799		11.655	1.00 21.92 1.00 21.36	E E
MOTA	4725	CB	PH			81.682		13.137	1.00 21.36 1.00 17.04	E
ATOM	4726					80.296		13.514	1.00 17.04	E
MOTA	4727					79.944 79.315		13.407 13.875	1.00 16.82	E
ATOM	4728					79.315 78.628			1.00 17.84	E
MOTA	4729					78.028			1.00 18.10	E
ATOM	4730			E E E E		77.661			1.00 16.61	E
ATOM	4731	L 4	EU	i £	, 10			27		

ATOM	4732	C	PHE	E	40	80.938	26.148	11.395	1.00 21.77	E
ATOM	4733	0	PHE	E	40	81.064	27.167	12.071	1.00 20.81	E
ATOM	4734	N	ASP	E	41	80.067	26.033	10.404	1.00 21.82	${f E}$
ATOM	4735	CA	ASP	E	41	79.181	27.110	9.995	1.00 21.76	E
ATOM	4736	CB	ASP	E	41	79.190	27.182	8.470	1.00 22.62	E
		CG	ASP	E	41	78.492	28.400	7.929	1.00 23.09	E
ATOM	4737				41	77.507	28.864	8.546	1.00 22.57	E
ATOM	4738	OD1	ASP	E				6.861	1.00 25.40	E
MOTA	4739	OD2	ASP	E	41	78.929	28.881			E
MOTA	4740	C	ASP	E	41	77.801	26.713	10.493	1.00 21.43	
ATOM	4741	0	ASP	E	41	77.277	25.672	10.085	1.00 22.83	E
MOTA	4742	N	SER	E	42	77.210	27.520	11.369	1.00 19.04	E
ATOM	4743	CA	SER	E	42	75.896	27.173	11.895	1.00 20.39	E
MOTA	4744	CB	SER	E	42	75.399	28.220	12.907	1.00 19.13	E
MOTA	4745	OG	SER	E	42	75.271	29.505	12.323	1.00 24.30	E
ATOM	4746	С	SER	E	42	74.891	27.000	10.762	1.00 20.23	E
ATOM	4747	0	SER	E	42	73.916	26.267	10.910	1.00 18.97	E
ATOM	4748	N	ASP	E	43	75.145	27.660	9.631	1.00 21.77	${f E}$
	4749	CA	ASP	E	43	74.261	27.556	8.470	1.00 24.99	E
ATOM			ASP	E	43	74.561	28.651	7.439	1.00 26.10	${f E}$
ATOM	4750	CB				73.819	29.947	7.727	1.00 28.71	E
ATOM	4751	CG	ASP	E	43		30.013	8.737	1.00 28.83	E
MOTA	4752	OD1		E 	43	73.078			1.00 20.05	E
ATOM	4753	OD2	ASP	E	43	73.976	30.902	6.939		E
ATOM	4754	С	ASP	E	43	74.378	26.193	7.809	1.00 25.68	
MOTA	4755	0	ASP	E	43	73.424	25.727	7.190	1.00 28.27	E
MOTA	4756	N	VAL	E	44	75.544	25.558	7.937	1.00 25.47	E
ATOM	4757	CA	VAL	E	44	75.764	24.229	7.362	1.00 23.51	E
ATOM	4758	CB	VAL	E	44	77.251	24.007	6.964	1.00 24.39	E
ATOM	4759	CG1	VAL	E	44	77.456	22.579	6.491	1.00 19.52	E
ATOM	4760	CG2	VAL	E	44	77.655	24.984	5.867	1.00 23.79	E
ATOM	4761	C	VAL		44	75.356	23.154	8.373	1.00 23.25	E
ATOM	4762	0	VAL		44	74.774	22.136	8.005	1.00 22.01	E
		И	GLY		45	75.683	23.370	9.644	1.00 22.52	E
ATOM	4763				4 5	75.292	22.411	10.664	1.00 21.82	E
ATOM	4764	CA	GLY				21.311	11.001	1.00 22.07	E
ATOM	4765	C	GLY		45	76.275			1.00 22.49	E
MOTA	4766	0	GLY		45	75.982	20.442	11.818		E
ATOM	4767	N	GLU		46	77.439	21.317	10.373	1.00 22.18	
MOTA	4768	CA	GLU	E	46	78.421	20.295	10.691	1.00 23.77	E
ATOM	4769	CB	GLU	E	46	78.147	19.017	9.891	1.00 26.29	E
ATOM	4770	CG	GLU	E	46	78.455	19.112	8.411	1.00 28.23	E
ATOM	4771	CD	GLU	E	46	78.214	17.795	7.677	1.00 32.67	E
ATOM	4772	OE1	GLU	E	46	78.575	17.706	6.482	1.00 33.19	E
ATOM	4773	OE2	GLU	E	46	77.661	16.855	8.290	1.00 33.19	${f E}$
ATOM	4774	C	GLÜ	E	46	79.807	20.839	10.383	1.00 23.15	E
ATOM	4775	Ō	GLU		46	79.943	21.880	9.747	1.00 23.06	E
ATOM	4776	N	PHE		47	80.835	20.153	10.857	1.00 21.79	E
	4777	CA	PHE		47	82.192	20.595	10.599	1.00 22.22	E
MOTA			PHE		47	83.175	19.864	11.515	1.00 22.30	E
ATOM	4778	CB			47	83.058	20.249	12.968	1.00 22.20	E
MOTA	4779	CG	PHE		•	83.867	21.246	13.508	1.00 19.80	E
MOTA	4780	CD1			47			13.802	1.00 23.06	E
MOTA	4781	CD2			47	82.151	19.598	14.858	1.00 18.93	E
MOTA	4782		PHE		47	83.781	21.585		1.00 22.63	E
ATOM	4783	CE2			47	82.055	19.931	15.157		E
MOTA	4784	CZ	PHE		47	82.872	20.925	15.684		
ATOM	4785	C	PHE	EE	47	82.513	20.278	9.147	1.00 24.14	E
ATOM	4786	0	PHE	E	47	82.064	19.258	8.609	1.00 23.25	E
MOTA	4787	N	ARG	E	48	83.272	21.164	8.511	1.00 22.66	E
MOTA	4788	CA	ARG	E	48	83.672	20.966	7.131	1.00 23.86	E
ATOM	4789	CB	ARG	E	48	82.801	21.795	6.181	1.00 23.48	E
ATOM	4790	CG	ARG	E	48	81.339	21.375	6.091	1.00 25.01	E
ATOM	4791	CD	ARC		48	81.155	20.061	5.348	1.00 25.08	E
ATOM	4792	NE	ARC			79.747	19.811	5.044	1.00 27.17	E
	4793	CZ	ARC		48	79.038	20.515	4.164	1.00 29.38	E
MOTA					48	79.604		3.498	1.00 31.36	E
ATOM	4794	CHN	_			77.763	20.226	3.946	1.00 30.50	E
MOTA	4795	NH2							1.00 24.13	E
MOTA	4796	C		3 E		85.119	21.395		1.00 25.58	E
ATOM	4797	0		E		85.507		7.416	1.00 23.36	E
ATOM	4798	N		A E		85.924	20.537	6.360		
MOTA	4799	CA		A E		87.316	20.875	6.122	1.00 23.11	E
MOTA	4800	CB	ALA	A E		88.102			1.00 22.46	E
MOTA	4801	C	AL	A E	49	87.290	21.875	4.980	1.00 22.04	E
MOTA	4802	0	AL	A E	49	86.507	21.722	4.048	1.00 23.16	E
ATOM	4803	N	VA	L E	50	88.108	22.916	5.050	1.00 23.56	E
MOTA	4804			L E		88.135	23.875	3.953	1.00 23.79	E
ATOM	4805	CB		L E		88.059	25.360	4.478	1.00 24.14	E
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ATOM	4806	CG1	VAL	E	50	88.341	25.408	5.959	1.00 24.71	E
ATOM	4807	CG2	VAL	E	50	89.010	26.268	3.704	1.00 22.47	E
ATOM	4808	C	VAL	E	50	89.374	23.578	3.098	1.00 23.50	E
ATOM	4809	0	VAL	E	50	89.485	24.041	1.963	1.00 24.92	E
ATOM	4810	N	THR		51	90.281	22.770	3.650	1.00 24.49	E
ATOM	4811	CA	THR		51	91.492	22.317	2.951	1.00 25.50	E
ATOM	4812	CB	THR		51	92.742	23.198	3.234	1.00 25.69	E
ATOM	4812	OG1	THR		51	93.171	23.007	4.586	1.00 27.89	E
		CG2	THR		51	92.443	24.670	2.985	1.00 23.29	E
ATOM	4814					91.817	20.895	3.420	1.00 26.59	E
ATOM	4815	C	THR		51				1.00 27.35	E
ATOM	4816	0	THR		51	91.387	20.477	4.496		E
ATOM	4817	N		E	52	92.576	20.154	2.617		
ATOM	4818	CA		E	52	92.949	18.783	2.956	1.00 28.49	E
ATOM	4819	CB		E	52		18.259	1.969	1.00 30.33	E
ATOM	4820	CG		E	52	93.536	17.892	0.556	1.00 34.17	E
ATOM	4821	CD1	LEU	E	52	94.749	17.628	-0.334	1.00 34.41	E
ATOM	4822	CD2	LEU	E	52	92.644	16.668	0.620	1.00 34.30	E
MOTA	4823	C	LEU	E	52	93.494	18.645	4.374	1.00 28.20	E
MOTA	4824	0	LEU	E	52	93.304	17.624	5.027	1.00 29.17	E
MOTA	4825	N	LEU	E	53	94.179	19.677	4.839	1.00 28.30	E
MOTA	4826	CA	LEU	E	53	94.766	19.682	6.171	1.00 28.75	E
MOTA	4827	CB	LEU	E	53	95.490	21.015	6.387	1.00 30.37	E
ATOM	4828	CG	LEU	E	53	96.939	21.010	6.882	1.00 32.74	E
ATOM	4829	CD1	LEU	E	53	97.777	20.085	6.008	1.00 31.60	E
ATOM	4830		LEU		53	97.498	22.444	6.854	1.00 30.06	E
ATOM	4831	C	LEU		53	93.727	19.464	7.278	1.00 27.82	E
ATOM	4832	0	LEU		53	94.027	18.858	8.312	1.00 25.47	E
ATOM	4833	N	GLY		5 4	92.508	19.957	7.059	1.00 27.39	E
ATOM	4834	CA	GLY		54	91.466	19.813	8.062	1.00 26.92	E
			GLY		5 4	90.569	18.589	7.949	1.00 28.33	E
ATOM	4835	C				89.725	18.348	8.813	1.00 28.02	E
ATOM	4836	0	GLY		54		17.801	6.898	1.00 20.02	E
MOTA	4837	N	LEU		55	90.755			1.00 25.28	E
ATOM	4838	CA	LEU		55	89.930	16.620	6.675		
MOTA	4839	CB	LEU		55	90.410	15.885	5.419	1.00 32.39	E
ATOM	4840	CG	LEU		55	89.426	14.934	4.731	1.00 35.68	E
ATOM	4841	CD1			55	88.086	15.627	4.504	1.00 34.41	E
ATOM	4842	CD2	LEU	E	55	90.018	14.473	3.406	1.00 35.99	E
MOTA	4843	C	LEU	E	55	89.865	15.659	7.867	1.00 32.09	E
MOTA	4844	0	LEU	\mathbf{E}	55	88.778	15.294	8.312	1.00 32.58	E
ATOM	4845	N	PRO	E	56	91.023	15.235	8.402	1.00 31.67	E
MOTA	4846	CD	PRO	E	56	92.411	15.520	8.000	1.00 31.37	E
ATOM	4847	CA	PRO	E	56	90.986	14.316	9.546	1.00 31.17	E
ATOM	4848	CB	PRO	E	56	92.459	14.163	9.919	1.00 30.50	E
ATOM	4849	CG	PRO	E	56	93.161	14.352	8.611	1.00 31.19	E
ATOM	4850	С	PRO	E	56	90.158	14.865	10.708	1.00 31.43	E
ATOM	4851	0	PRO		56	89.250	14.195	11.205	1.00 32.17	E
ATOM	4852	N	ALA		57	90.473	16.086	11.138	1.00 29.94	E
ATOM	4853	CA	ALA		57	89.748	16.709	12.244	1.00 28.45	E
ATOM	4854	CB	ALA		57	90.314	18.098	12.532	1.00 27.09	E
ATOM	4855	C	ALA		5 <i>7</i>	88.249	16.807	11.960	1.00 27.57	E
	4856	0	ALA		5 <i>7</i>	87.436	16.466	12.812	1.00 26.57	E
ATOM			ALA		58	87.899	17.270	10.761	1.00 27.40	E
ATOM	4857	N					17.422	10.349	1.00 28.85	E
ATOM	4858	CA	ALA		58	86.505		8.939	1.00 27.80	E
MOTA	4859	CB	ALA		58	86.439	18.007		1.00 27.80	E
MOTA	4860	C	ALA		58	85.726	16.110	10.406		
ATOM	4861	0	ALA		58	84.624	16.058	10.954	1.00 29.58	E
ATOM	4862	N	GLU		59	86.292	15.052	9.837	1.00 32.24	E
MOTA	4863	CA	GLŪ		59	85.632	13.750	9.845	1.00 35.22	E
MOTA	4864	CB	GLU	E	59	86.441	12.724	9.049	1.00 36.81	E
MOTA	4865	CG	GLU	\mathbf{E}	59	86.392	12.917	7.549	1.00 40.89	. E
MOTA	4866	CD	GLU	E	59	87.057	11.775	6.805	1.00 44.28	E
ATOM	4867	OE1	GLU	E	59	88.291	11.597	6.955	1.00 45.76	${f E}$
ATOM	4868	OE2	GLU	E	59	86.342	11.052	6.075	1.00 45.12	E
ATOM	4869	C	GLU	E	59	85.441	13.231	11.260	1.00 34.08	E
ATOM	4870	0	GLU		59	84.384	12.697	11.596	1.00 34.48	E
ATOM	4871	N	TYR		60	86.466	13.387	12.090	1.00 33.21	E
ATOM	4872	CA	TYR		60	86.390	12.919	13.463	1.00 32.36	E
ATOM	4873	CB	TYR		60	87.724	13.101	14.177	1.00 33.78	E
ATOM	4874	CG	TYR		60	87.657	12.617	15.594	1.00 35.68	E
ATOM	4874	CD1			60	87.543	11.259	15.872	1.00 37.48	E
		CE1			60	87.394	10.802	17.173	1.00 41.14	E
MOTA	4876				60	87.628	13.514	16.655	1.00 37.26	E
MOTA	4877	CD2			60		13.073	17.965	1.00 37.26	E
ATOM	4878	CE2				87.478			1.00 40.26	E
MOTA	4879	CZ	TYR	ഥ	б0	87.360	11.714	18.218	T.00 #T.00	Ţ

ATOM	4880	OH	TYR	E	60	87.198	11.262	19.508	1.00 44.51	${f E}$
ATOM	4881	C	TYR		60	85.312	13.623	14.275	1.00 32.30	E
	4882	0	TYR		60	84.430	12.976	14.839	1.00 30.56	E
ATOM									1.00 31.42	E
ATOM	4883	N		E	61	85.391	14.950	14.347		
ATOM	4884	CA	TRP	E	61	84.412	15.715	15.112	1.00 31.35	E
ATOM	4885	CB	TRP	E	61	84.744	17.219	15.071	1.00 32.78	E
ATOM	4886	CG	TRP	E	61	86.051	17.584	15.748	1.00 35.14	E
ATOM	4887	CD2	TRP	E	61	86.909	18.687	15.425	1.00 37.07	E
ATOM	4888	CE2		E	61	87.994	18.655	16.331	1.00 37.15	${f E}$
							19.706	14.458	1.00 39.50	E
ATOM	4889	CE3	TRP	E	61	86.864				
ATOM	4890	CD1	TRP	E	61	86.635	16.947	16.809	1.00 35.82	E
ATOM	4891	NE1	TRP	E	61	87.800	17.582	17.163	1.00 35.66	E
ATOM	4892	CZ2	TRP	E	61	89.034	19.602	16.300	1.00 38.95	E
ATOM	4893	CZ3	TRP	E	61	87.902	20.656	14.427	1.00 41.16	E
ATOM	4894	CH2	TRP	E	61	88.971	20.591	15.346	1.00 40.81	E
		C	TRP	E	61	82.968	15.472	14.653	1.00 29.29	E
ATOM	4895									E
ATOM	4896	0	TRP	E	61	82.045	15.563	15.458		
ATOM	4897	N	ASN	E	62	82.772	15.162	13.373	1.00 27.86	E
ATOM	4898	CA	ASN	E	62	81.428	14.902	12.853	1.00 29.09	${f E}$
ATOM	4899	CB	ASN	\mathbf{E}	62	81.379	15.051	11.331	1.00 29.42	E
ATOM	4900	CG	ASN	E	62	81.241	16.492	10.893	1.00 31.22	${f E}$
ATOM	4901	OD1	ASN	E	62	80.563	17.288	11.545	1.00 29.56	E
						81.870	16.834	9.772	1.00 31.73	E
ATOM	4902	ND2		E	62					E
ATOM	4903	C		\mathbf{E}	62	80.906	13.519	13.220	1.00 28.26	
MOTA	4904	0	ASN	E	62 ,	79.716	13.242	13.086	1.00 27.48	E
ATOM	4905	N	SER	${f E}$	63	81.795	12.647	13.672	1.00 27.47	${f E}$
ATOM	4906	CA	SER	E	63	81.381	11.311	14.056	1.00 29.39	E
ATOM	4907	CB	SER		63	82.511	10.310	13.803	1.00 28.56	${f E}$
	4908	OG	SER		63	83.607	10.545	14.671	1.00 32.72	E
ATOM						80.987	11.310	15.534	1.00 30.11	E
MOTA	4909	C	SER		63					E
MOTA	4910	0	SER		63	80.515	10.297	16.055	1.00 31.52	
MOTA	4911	N	GLN	E	64	81.173	12.453	16.196	1.00 28.86	E
ATOM	4912	CA	GLN	E	64	80.834	12.604	17.612	1.00 28.28	E
ATOM	4913	CB	GLN	E	64	81.929	13.379	18.350	1.00 29.50	E
MOTA	4914	CG	GLN	E	64	83.330	12.787	18.266	1.00 29.72	E
ATOM	4915	CD			64	83.418	11.412	18.888	1.00 32.69	E
			GLN		64	83.055	10.405	18.267	1.00 35.22	E
ATOM	4916	OE1					11.358	20.128	1.00 31.92	E
MOTA	4917	NE2	GLN		64	83.887				
MOTA	4918	C	GLN		64	79.522	13.366	17.783	1.00 28.42	E
MOTA	4919	0	GLN	E	64	79.525	14.599	17.800	1.00 27.68	E
ATOM	4920	N	LYS	${f E}$	65	78.410	12.648	17.926	1.00 27.17	E
ATOM	4921	CA	LYS	E	65	77.111	13.300	18.097	1.00 29.82	${f E}$
ATOM	4922	CB	LYS	E	65	75.994	12.258	18.253	1.00 31.43	E
ATOM	4923	CG	LYS		65	75.479	11.692	16.936	1.00 37.61	E
						74.801	12.766	16.072	1.00 41.12	E
MOTA	4924	CD	LYS		65 65				1.00 44.25	E
ATOM	4925	CE	LYS		65	73.489	13.267	16.696		
MOTA	4926	NZ	LYS	E	65	72.832	14.322	15.861	1.00 44.10	E
ATOM	4927	C	LYS	${f E}$	65	77.067	14.273	19.278	1.00 28.07	E
ATOM	4928	0	LYS	E	65	76.406	15.308	19.211	1.00 27.46	E
ATOM	4929	N	ASP	E	66	77.758	13.938	20.361	1.00 27.40	${f E}$
MOTA	4930	CA	ASP		66	77.783	14.809	21.532	1.00 26.85	E
			ASP		66	78.566	14.142	22.670	1.00 26.10	E
ATOM	4931	CB						22.212	1.00 29.25	E
MOTA	4932	CG	ASP		66	79.899	13.576			
MOTA	4933	OD1	ASP	E	66	79.915	12.836	21.205	1.00 28.95	E
MOTA	4934	OD2	ASP	${f E}$	66	80.929	13.858	22.864	1.00 31.03	E
ATOM	4935	C	ASP	E	66	78.390	16.174	21.193	1.00 26.21	E
MOTA	4936	0	ASP	E	66	77.844	17.215	21.559	1.00 26.58	E
ATOM	4937	N	ILE		67	79.510	16.170	20.478	1.00 26.25	E
		CA	ILE		67	80.164	17.414	20.100	1.00 25.76	E
MOTA	4938							19.477	1.00 27.31	E
MOTA	4939	CB	ILE		67	81.551	17.153			
MOTA	4940	CG2	ILE		67	82.261	18.467	19.210	1.00 25.90	E
MOTA	4941	CG1	ILE	\mathbf{E}	67	82.396	16.304	20.429	1.00 28.85	E
MOTA	4942	CD1	ILE	E	67	82.494	16.871	21.844	1.00 32.35	${f E}$
ATOM	4943	C	ILE	E	67	79.307	18.189	19.108	1.00 25.95	E
ATOM	4944	Ō	ILE		67	79.125	19.392	19.255	1.00 26.97	E
ATOM	4945	N	LEU		68	78.775	17.504	18.100	1.00 26.05	E
						77.927	18.172	17.113	1.00 26.36	E
ATOM	4946	CA	LEU		68				1.00 26.91	E
ATOM	4947	CB	LEU		68	77.382	17.169	16.094		
MOTA	4948	CG	LEU		68	78.154	16.987	14.790	1.00 27.01	E
ATOM	4949	CD1			68	77.389	16.002	13.913	1.00 26.26	E
MOTA	4950	CD2	LEU	E	68	78.311	18.342	14.076	1.00 24.04	\mathbf{E}
ATOM	4951	C	LEU	E	68	76.760	18.870	17.792	1.00 26.03	E
ATOM	4952	0	LEU		68	76.433	20.011	17.465	1.00 25.76	\mathbf{E}
ATOM	4953	N	GLU		69	76.134	18.175	18.737	1.00 27.50	E
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ATOM	4954	CA	GLU	E	69	75.000	18.726	19.471	1.00	30.38	E
ATOM	4955	CB	GLU	F.	69	74.481	17.720	20.508	1.00	34.06	E
ATOM	4956	CG	GLU		69	73.426	16.742	19.989	1.00	40.55	E
ATOM	4957	CD	GLU		69	72.211	17.444	19.392	1.00	44.43	E
ATOM	4958	OE1	GLU	E	69	71.802	18.505	19.922	1.00	43.73	E
ATOM	4959	OE2	GLU	E	69	71.656	16.926	18.397	1.00	48.15	E
ATOM	4960	С	GLU	F:	69	75.335	20.034	20.178	1.00	29.17	E
			GLU		69		21.009	20.071	1.00	29.71	E
ATOM	4961	0				74.587					
ATOM	4962	N	ARG		70	76.453	20.059	20.899	1.00	26.65	E
ATOM	4963	CA	ARG	\mathbf{E}	70	76.844	21.262	21.620	1.00	25.51	E
MOTA	4964	CB	ARG	E	70	78.001	20.965	22.572	1.00	27.14	E
ATOM	4965	CG		E	70	77.711	19.855	23.563	1.00	31.22	E
ATOM	4966	CD	ARG		70	78.637	19.934	24.769	1.00	35.11	E
ATOM	4967	NE	ARG	E	70	78.758	18.647	25.440	1.00	39.19	E
ATOM	4968	CZ	ARG	E	70	79.456	17.628	24.956	1.00	41.08	E
ATOM	4969	NH1	ARG	E	70	80.096	17.752	23.802	1.00	45.32	${f E}$
ATOM	4970	NH2	ARG	E	70	79.511	16.486	25.618	1.00	44.01	E
					70	77.230	22.395	20.677	1.00	24.57	E
ATOM	4971	C		E							
ATOM	4972	0	ARG	E	70	76.927	23.557	20.941	1.00	21.44	E
ATOM	4973	N	LYS	\mathbf{E}	71	77.897	22.057	19.576	1.00	24.56	${f E}$
ATOM	4974	CA	LYS	E	71	78.309	23.071	18.612	1.00	24.08	E
ATOM	4975	CB	LYS	E	71	79.202	22.452	17.534	1.00	25.39	E
		CG		E	71	80.100	23.474	16.852	1.00	29.73	E
ATOM	4976										
ATOM	4977	CD		E	71	81.067	24.095	17.862	1.00	30.94	E
ATOM	4978	CE	LYS	E	71	81.905	25.205	17.256	1.00	31.82	E
ATOM	4979	NZ	LYS	E	71	82.774	25.849	18.290	1.00	33.45	E
ATOM	4980	C	LYS	E	71	77.087	23.732	17.960	1.00	22.42	E
ATOM	4981			E	71	77.045	24.951	17.780	1.00	18.65	E
		0									
ATOM	4982	N		E	72	76.092	22.919	17.620	1.00	22.31	E
ATOM	4983	CA	ARG	\mathbf{E}	72	74.867	23.419	17.002	1.00	21.44	${f E}$
MOTA	4984	CB	ARG	E	72	73.984	22.250	16.578	1.00	19.93	E
ATOM	4985	CG	ARG	E	72	74.534	21.497	15.407	1.00	21.45	E
ATOM	4986	CD	ARG		72	73.779	20.223	15.141	1.00	23.34	E
ATOM	4987	NE	ARG		72	74.211	19.643	13.877	1.00	24.99	E
MOTA	4988	CZ	ARG	E	72	74.028	18.377	13.522	1.00	27.42	${f E}$
MOTA	4989	NHl	ARG	E	72	73.411	17.533	14.344	1.00	25.90	${f E}$
ATOM	4990	NH2	ARG	E	72	74.475	17.955	12.341	1.00	25.41	E
ATOM	4991	C		E	72	74.093	24.315	17.961	1.00	21.34	E
										23.67	E
ATOM	4992	0		E	72	73.336	25.182	17.535	1.00		
ATOM	4993	N	ALA	E	73	74.293	24.105	19.256	1.00	21.13	E
MOTA	4994	CA	ALA	E	73	73.610	24.887	20.281	1.00	22.11	E
MOTA	4995	CB	ALA	E	73	73.476	24.052	21.568	1.00	21.20	E
ATOM	4996	C	ALA	E	73	74.347	26.189	20.576	1.00	22.67	E
			ALA		73	73.773	27.133	21.125	1.00	25.58	E
MOTA	4997	0									
MOTA	4998	N	ALA		74	75.614	26.248	20.195	1.00	22.52	E
MOTA	4999	CA	ALA	\mathbf{E}	74	76.420	27.432	20.448	1.00	22.20	E
ATOM	5000	CB	ALA	E	74	77.830	27.219	19.910	1.00	24.81	E
MOTA	5001	C	ALA	E	74	75.828	28.722	19.882	1.00	22.28	E
ATOM	5002	0	ALA		74	76.027	29.796	20.452	1.00	20.24	E
											E
ATOM	5003	N	VAL		75	75.102	28.634	18.770		21.92	
ATOM	5004	CA	VAL	E	75	74.519	29.841	18.185	1.00	21.69	E
MOTA	5005	CB	VAL	E	75	73.700	29.517	16.890	1.00	22.61	E
ATOM	5006	CG1	VAL	E	75	72.488	28.657	17.219	1.00	24.39	${f E}$
ATOM	5007	CG2	VAL	E	75	73.270	30.798	16.218	1.00	24.00	E
ATOM	5008	C	VAL		75	73.639	30.558	19.219	1.00	21.26	E
MOTA	5009	0	JAV		75	73.464	31.777	19.164	1.00	20.64	E
MOTA	5010	N	ASP	\mathbf{E}	76	73.106	29.802	20.171	1.00	20.84	E
MOTA	5011	CA	ASP	E	76	72.273	30.385	21.220	1.00	23.98	E
ATOM	5012	CB	ASP	E	76	71.022	29.532	21.471	1.00	25.33	E
ATOM	5013	CG	ASP		76	70.010	29.605	20.331		27.46	$oldsymbol{\mathrm{E}}$
-								19.763			
MOTA	50,14	OD1	ASP		76	69.807	30.697			29.45	E .
MOTA	5015	OD2	ASP		76	69.398	28.566	20.020		31.17	E
MOTA	5016	C	ASP	E	76	73.044	30.525	22.538	1.00	24.46	E
ATOM	5017	0	ASP	E	76	72.910	31.524	23.247	1.00	25.64	E
ATOM	5018	N	ARG		77	73.846	29.515	22.855		23.56	E
	5019	CA	ARG		77	74.627	29.486	24.085		22.99	E
ATOM											
ATOM	5020	CB	ARG		77	75.176	28.077	24.279		26.55	E
ATOM	5021	CG	ARG		77	75.848	27.806	25.607		33.45	E
ATOM	5022	CD	ARG	E	77	75.961	26.295	25.825	1.00	37.66	E
ATOM	5023	NE	ARG	E	77	74.639	25.666	25.883	1.00	40.99	E
ATOM	5024	CZ	ARG		77	74.423	24.352	25.862		43.13	E
100,000	5025	NH1			77	75.438	23.503	25.782		43.11	E
ATOM											
MOTA	5026	NH2	ARG		77	73.183	23.885	25.914		44.93	E
MOTA	5027	C	ARG	E	77	75.763	30.509	24.078	1.00	23.23	E

ATOM	5028	0	ARO	S E	77	76.162	31.022	25.129	1.00 23.14	E
ATOM	5029	N	VAI	E	78	76.275	30.808		1.00 20.54	E
MOTA	5030	CA	VAI	E	78	77.354	31.767		1.00 19.56	E
ATOM	5031	CB	VAI	E	78	78.500	31.181		1.00 19.17	E
ATOM	5032	CG1	L VAI	E	78	79.612	32.208	21.724	1.00 17.69	E
ATOM	5033	CG2	IAV S	E	78	79.032	29.921		1.00 19.40	E
ATOM	5034	C	VAI	E		76.888	33.075	22.093	1.00 19.95	E
ATOM	5035	0	VAI			76.786	34.110	22.756	1.00 21.57	
ATOM	5036	N	CYS			76.595	33.021	20.799	1.00 21.57	E
ATOM	5037	CA	CYS			76.181	34.205	20.799		E
ATOM	5038	C	CYS			74.967			1.00 17.48	E
ATOM	5039	0	CYS		· -		34.966	20.620	1.00 18.40	E
ATOM	5040	CB	CYS			75.087	36.146	20.967	1.00 16.69	E
ATOM	5041	SG	CYS		· -	75.946	33.847	18.592	1.00 17.30	E
ATOM	5042	N	ARG		_	77.361	33.071	17.722	1.00 27.04	E
MOTA	5042				80	73.802	34.326	20.717	1.00 17.59	E
ATOM		CA	ARG			72.641	35.050	21.240	1.00 20.01	E
	5044	CB	ARG		80	71.340	34.256	21.032	1.00 20.22	E
MOTA	5045	CG	ARG			70.886	34.213	19.584	1.00 22.92	E
ATOM	5046	CD	ARG		80	69.423	33.811	19.439	1.00 23.91	E
ATOM	5047	NE	ARG		80	68.972	33.965	18.057	1.00 23.49	E
ATOM	5048	CZ	ARG		80	69.206	33.089	17.082	1.00 25.16	E
ATOM	5049	NHl			80	69.884	31.975	17.326	1.00 24.15	E
MOTA	5050	NH2			80	68.778	33.336	15.851	1.00 25.51	E
ATOM	5051	С	ARG	E	80	72.804	35.423	22.716	1.00 20.35	E
ATOM	5052	0	ARG	E	80	72.317	36.464	23.153	1.00 17.98	E
ATOM	5053	N	HIS	E	81	73.495	34.581	23.479	1.00 21.22	E
ATOM	5054	CA	HIS	E	81	73.717	34.867	24.895	1.00 22.79	E
MOTA	5055	CB	HIS	E	81	74.467	33.717	25.572	1.00 24.38	E
ATOM	5056	CG	HIS	E	81	74.955	34.046	26.950	1.00 26.42	E
ATOM	5057	CD2	HIS	E	81	76.188	34.381	27.404	1.00 26.61	E
ATOM	5058	ND1	HIS	\mathbf{E}	81	74.122	34.080	28.048	1.00 26.60	E
ATOM	5059	CE1	HIS	E	81	74.819	34.420	29.117	1.00 25.75	E
ATOM	5060	NE2	HIS	E	81	76.075	34.609	28.754	1.00 26.16	E
ATOM	5061	C	HIS	E	81	74.531	36.146	25.060	1.00 21.41	E
ATOM	5062	0	HIS		81	74.109	37.076	25.742	1.00 19.84	E
ATOM	5063	N	ASN		82	75.700	36.188	24.426	1.00 22.13	E
ATOM	5064	CA	ASN		82	76.568	37.361	24.535	1.00 22.13	E
ATOM	5065	CB	ASN		82	77.927	37.111	23.864	1.00 21.51	
ATOM	5066	CG	ASN		82	78.702	35.982	24.515		E
ATOM	5067	OD1			82	78.453	35.632	25.669		E
ATOM	5068	ND2			82	78. 4 55			1.00 19.05	E
ATOM	5069	C	ASN		82		35.409	23.777	1.00 15.06	E
ATOM	5070	0	ASN			75.936	38.612	23.949	1.00 20.33	E
ATOM	5071	И			82	76.212	39.716	24.412	1.00 22.84	E
ATOM	5072		TYR		83	75.089	38.454	22.940	1.00 19.71	E
ATOM		CA	TYR		83	74.454	39.620	22.336	1.00 20.96	E
MOTA	5073	CB	TYR		83	73.619	39.211	21.114	1.00 21.58	E
	5074	CG	TYR		83	73.223	40.368	20.218	1.00 22.56	E
ATOM	5075	CD1	TYR		83	72.047	41.090	20.439	1.00 23.70	E
MOTA	5076	CE1	TYR		83	71.682	42.152	19.593	1.00 25.46	E
ATOM	5077	CD2			83	74.027	40.736	19.140	1.00 22.35	E
ATOM	5078	CE2	TYR		83	73.675	41.788	18.297	1.00 24.48	E
ATOM	5079	CZ	TYR		83	72.508	42.491	18.523	1.00 26.06	E
ATOM	5080	OH	TYR		83	72.185	43.524	17.671	1.00 28.63	E
ATOM	5081	C	TYR		83	73.583	40.345	23.363	1.00 21.22	E
MOTA	5082	0	TYR	E	83	73.399	41.557	23.276	1.00 21.25	E
ATOM	5083	N	GLN	E	84	73.046	39.606	24.333	1.00 22.94	E
MOTA	5084	CA	GLN	E	84	72.234	40.226	25.377	1.00 25.07	E
ATOM	5085	CB	GLN	E	84	71.631	39.180	26.324	1.00 25.76	E
ATOM	5086	CG	${ t GLN}$	\mathbf{E}	84	70.863	38.047	25.653	1.00 30.97	E
ATOM	5087	CD	GLN	E	84	69.889	38.525	24.594	1.00 33.95	E
ATOM	5088	OE1	GLN	E	84	69.055	39.401	24.840	1.00 36.35	E
MOTA	5089	NE2	GLN	E	84	69.986	37.940	23.401	1.00 36.25	E
ATOM	5090	C		E	84	73.158	41.145	26.174	1.00 25.41	E
ATOM	5091	0	GLN	E	84	72.804	42.290	26.473	1.00 27.11	E
MOTA	5092	N		E	85	74.344	40.637	26.510	1.00 27.11	E
ATOM	5093	CA		E	85	75.330	41.413			
ATOM	5094	CB		E	85 85	75.330 76.601		27.256	1.00 26.47	E
ATOM	5095	CG		E			40.590	27.515	1.00 26.91	E
ATOM ATOM	5096			E	85 85	76.485	39.202	28.161	1.00 29.65	E
ATOM	5097			-	85 85	77.872	38.735	28.587	1.00 31.29	E
ATOM ATOM	5097			E	85 05	75.564	39.247	29.365	1.00 32.27	E
ATOM ATOM		C		E	85 85	75.698	42.661	26.459	1.00 26.89	E
	5099 5100	O NT		E	85	75.762	43.757	27.004	1.00 28.24	E
ATOM ATOM	5100	N		E	86	75.941	42.484	25.162	1.00 27.39	E
ATOM	5101	CA	GLU	E	86	76.293	43.603	24.295	1.00 28.02	E

ATOM	5102	CB	GLU E	86	76.492	43.126	22.852	1.00 26.60	E
MOTA	5103	CG	GLU E	86	77.524	42.026	22.672	1.00 30.65	E
MOTA	5104	CD	GLU E	86	78.942	42.457	23.024	1.00 31.17	E
MOTA	5105	OE1	GLU E	86	79.860	41.612	22.919	1.00 31.68	E
ATOM	5106	OE2	GLU E	86	79.139	43.631	23.402	1.00 31.77	E
ATOM	5107	C	GLU E	86	75.165	44.630	24.327	1.00 27.95	E
MOTA	5108	0	GLU E	86	75.407	45.834	24.257	1.00 24.30	E
ATOM	5109	Ŋ	LEU E	87	73.935	44.130	24.442	1.00 28.96	E
ATOM	5110	CA	LEU E	87	72.736	44.962	24.468	1.00 32.20	E
ATOM	5111	CB	LEU E	87	71.496	44.062	24.423	1.00 32.64	E
ATOM	5112	CG	LEU E	87	70.506	44.100	23.248	1.00 35.59	E
ATOM	5113	CD1	LEU E	87	71.101	44.734	21.997	1.00 35.24	E
MOTA	5114	CD2	LEU E	87	70.071	42.675	22.965	1.00 34.35	E
ATOM	5115	C	LEU E	87	72.669	45.893	25.686	1.00 33.33	E
ATOM	5116	0	LEU E	87	71.967	46.902	25.663	1.00 32.52	E
ATOM	5117	N	ARG E	88	73.401	45.560	26.745	1.00 35.06	E
ATOM	5118	CA	ARG E	88	73.399	46.389	27.948	1.00 37.29	E
ATOM	5119	CB	ARG E	88	73.348	45.524	29.215	1.00 39.69	E
ATOM	5120	ÇG	ARG E	88	72.471	44.275	29.158	1.00 43.37	E
ATOM	5121	CD	ARG E	88	72.441	43.592	30.529	1.00 45.38	E
ATOM	5122	NE	ARG E	88	71.846	42.257	30.499	1.00 48.76	E
MOTA	5123	CZ	ARG E	88	70.625	41.985	30.047	1.00 50.95	E
ATOM	5124	NH1	ARG E	88	69.854	42.958	29.579	1.00 52.23	E
ATOM	5125	NH2	ARG E	88	70.171	40.738	30.064	1.00 51.26	E
ATOM	5126	C	ARG E	88	74.670	47.225	28.010	1.00 37.36	E
ATOM	5127	0	ARG E	88	74.842	48.044	28.913	1.00 37.55	E
ATOM	5128	N	THR E	89	75.564	47.019	27.049	1.00 36.40	\mathbf{E}
MOTA	5129	CA	THR E	89	76.834	47.731	27.055	1.00 34.93	E
MOTA	5130	CB	THR E	89	77.951	46.807	27.590	1.00 36.26	E
MOTA	5131	OG1	THR E	89	77.973	45.590	26.825	1.00 34.21	E
ATOM	5132	CG2	THR E	89	77.708	46.478	29.056	1.00 33.95	E
MOTA	5133	C	THR E	89	77.294	48.304	25.718	1.00 33.37	E
MOTA	5134	0	THR E	89	76.958	49.431	25.356	1.00 33.30	E
MOTA	5135	N	THR E	90	78.080	47.510	25.000	1.00 32.11	E
MOTA	5136	CA	THR E	90	78.639	47.895	23.712	1.00 30.45	E
ATOM	5137	CB	THR E	90	79.313	46.681	23.041	1.00 31.20	E
MOTA	5138	OG1	THR E	90	80.238	46.086	23.958	1.00 32.67	E
ATOM	5139	CG2	THR E	90	80.076	47.109	21.811	1.00 32.64	E
MOTA	5140	C	THR E	90	77.639	48.504	22.738	1.00 28.40	E
MOTA	5141	0	THR E	90	77.903	49.538	22.133	1.00 27.20	E
MOTA	5142	N	LEU E	91	76.489	47.864	22.582	1.00 29.83	E
MOTA	5143	CA	LEU E	91	75.482	48.361	21.655	1.00 29.52	E
MOTA	5144	CB	LEU E	91	74.474	47.252	21.354	1.00 27.50	E
MOTA	5145	CG	LEU E	91	75.091	46.101	20.550	1.00 26.15	E
ATOM	5146	CD1	LEU E	91	74.102	44.959	20.457	1.00 24.51	E
MOTA	5147	CD2		91	75.487	46.593	19.157	1.00 23.04	E
ATOM	5148	C	LEU E	91	74.770	49.629	22.129	1.00 30.74	E
MOTA	5149	0	LEU E	91	73.994	50.228	21.382	1.00 31.46	E
ATOM	5150	N	GLN E	92	75.035	50.043	23.366	1.00 29.33	E
ATOM	5151	CA	GLN E	92	74.427	51.259	23.884	1.00 30.04	E
ATOM	5152	CB	GLN E	92	73.869	51.044	25.294	1.00 31.55	E
ATOM	5153	CG	GLN E	92	72.500	50.381	25.327	1.00 36.90	E
ATOM	5154	CD	GLN E	92	71.865	50.426	26.706	1.00 41.59	E
ATOM	5155	OE1		92	70.760	49.920	26.911	1.00 43.76	E E
ATOM	5156	NE2		92	72.563	51.037 52.409	27.662	1.00 43.75 1.00 28.45	E
ATOM	5157	C	GLN E	92	75.430		23.898		E
ATOM	5158	0	GLN E	92	75.059	53.558	24.125 23.650		E
ATOM	5159	N	ARG E	93	76.699	52.098		1.00 26.37 1.00 26.74	E
ATOM	5160	CA	ARG E	93	77.737	53.127 52.513	23.633 23.340	1.00 28.74	E
ATOM	5161	CB	ARG E	93	79.112	53.525	23.340	1.00 24.84	E
ATOM	5162	CG	ARG E	93	80.260	52.801	22.894	1.00 20.15	E
ATOM	51.63	CD	ARG E	93	81.569	53.685	22.729	1.00 20.08	E
ATOM	5164	NE	ARG E	93	82.718	54.330	23.729	1.00 15.27	E
MOTA	5165	CZ	ARG E	93	83.316 82.875	54.197	24.973	1.00 16.93	E
ATOM	5166 5167	NH1		93	82.875	55.101	24.973	1.00 17.82	E
ATOM	5167 5169	NH2		93 93	77.428	54.173	23.492	1.00 18.26	E
ATOM	5168 5169	C O	ARG E	93	77.428	53.847	21.407	1.00 28.20	E
ATOM ATOM	5170	И	ARG E	93	77.202	55.431	22.995	1.00 23.30	E
ATOM	5171	CA	ARG E	94	77.411	56.529	22.084	1.00 20.24	E
ATOM	5172	CB	ARG E	94	75.661	56.855	22.053	1.00 32.88	E
ATOM	5172	CG	ARG E	94	74.912	55.941	21.086	1.00 32.00	E
ATOM	5174	CD	ARG E	94	73.402	56.055	21.163	1.00 40.38	E
MOTA	5175	NE	ARG E	94	72.758	55.304	20.080	1.00 44.16	E
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ATOM	5176	CZ	ARG	E	94	72.871	53.991	19.894	1.00 43.57	E
ATOM	5177	NH1	ARG	E	94	73.602	53.259	20.720	1.00 45.04	E
MOTA	5178	NH2	ARG	E	94	72.262	53.408	18.869	1.00 45.75	E
MOTA	5179	C	ARG	E	94	77.992	57.734	22.497	1.00 29.26	E
ATOM	5180	0	ARG	E	94	77.773	58.331	23.546	1.00 30.32	E
MOTA	5181	N	VAL	E	95	78.974	58.063	21.667	1.00 26.76	E
ATOM	5182	CA	VAL	E	95	79.859	59.188	21.936	1.00 25.75	E
ATOM	5183	CB	VAL	E	95	81.340	58.763	21.855	1.00 22.33	E
MOTA	5184	CG1	VAL	E	95	82.244	59.914	22.287	1.00 19.80	E
ATOM	5185	CG2	VAL	E	95	81.565	57.534	22.717	1.00 19.11	E
ATOM	5186	C	VAL	E	95	79.600	60.266	20.902	1.00 26.51	E
MOTA	5187	0	VAL	E	95	79.787	60.042	19.703	1.00 27.04	E
ATOM	5188	N			96	79.160	61.430	21.366	1.00 27.28	E
ATOM	5189	CA	GLU		96	78.870	62.536	20.466	1.00 28.16	E
ATOM	5190	CB	GLU		96	78.260	63.716	21.227	1.00 30.40	E
ATOM	5191	CG	GLU		96	76.965	63.396	21.952	1.00 34.36	E
ATOM	5192	CD	GLU		96	76.348	64.625	22.609	1.00 36.84	E
ATOM	5193	OE1	GLU		96	75.295	64.478	23.272	1.00 38.81	E
MOTA	5194	OE2	GLU		96 26	76.914	65.734	22.460	1.00 35.73	E
MOTA	5195	C	GLU		96 06	80.148	62.987	19.793	1.00 25.65	E
ATOM	5196	0	GLU		96 07	81.176	63.171	20.440	1.00 24.93	E
ATOM	5197 5198	N CD	PRO PRO		97 97	80.101 78.977	63.168 62.979	18.473 17.539	1.00 25.41 1.00 24.36	E E
ATOM ATOM	5199	CA	PRO		97 97	81.304	63.603	17.770	1.00 24.81	E
ATOM	5200	CB	PRO		97 97	80.927	63.416	16.306	1.00 24.81	E
ATOM	5200	CG	PRO		97 97	79.456	63.717	16.309	1.00 24.85	E
ATOM	5201	C	PRO		97	81.643	65.048	18.089	1.00 23.30	E
ATOM	5202	0	PRO		97	80.761	65.844	18.419	1.00 23.85	E
ATOM	5204	N	THR		98	82.927	65.377	18.025	1.00 22.82	E
MOTA	5205	CA	THR		98	83.340	66.748	18.244	1.00 24.12	E
ATOM	5206	CB	THR		98	84.679	66.852	19.019	1.00 26.31	E
ATOM	5207	OG1	THR		98	85.744	66.355	18.205	1.00 34.47	E
ATOM	5208	CG2	THR		98	84.623	66.049		1.00 23.83	E
MOTA	5209	C	THR	E	98	83.519	67.254	16.817	1.00 22.12	E
ATOM	5210	0	THR	E	98	84.162	66.601	15.993	1.00 21.35	E
ATOM	5211	N	VAL	E	99	82.923	68.400	16.516	1.00 21.99	E
MOTA	5212	CA	VAL	E	99	83.001	68.957	15.177	1.00 20.67	E
ATOM	5213	CB	VAL	E	99	81.585	69.217	14.619	1.00 19.57	E
ATOM	5214	CG1	VAL	E	99	81.667	69.645	13.154	1.00 14.62	E
MOTA	5215	CG2	VAL	E	99	80.732	67.944	14.766	1.00 15.20	E
ATOM	5216	C	VAL	E	99	83.814	70.240	15.158	1.00 22.05	E
MOTA	5217	0	VAL	E	99	83.524	71.194	15.884	1.00 22.27	E
ATOM	5218	N	THR		100	84.827	70.250	14.304	1.00 21.34	E
ATOM	5219	CA	THR		100	85.728	71.376	14.176	1.00 23.10	E
ATOM	5220	CB	THR		100	87.104	71.024	14.786	1.00 24.55	E
MOTA	5221	OG1	THR		100	86.941	70.728	16.180	1.00 30.47	E
ATOM	5222	CG2	THR		100	88.079	72.183	14.634	1.00 27.79	E
ATOM	5223	C	THR		100	85.934	71.777	12.722	1.00 23.36	E
ATOM	5224	0	THR		100	86.024	70.926	11.842	1.00 21.77	E E
ATOM	5225 5226	N C7	ILE		101	86.009 86.236	73.082 73.584	12.473 11.124	1.00 24.40 1.00 25.31	E
ATOM ATOM	5226 5227	CA CB	ILE		101	85.092	74.518	10.645	1.00 23.31	E
ATOM	5228	CG2	ILE		101	85.398	75.044	9.245	1.00 24.21	E
ATOM	5229	CG1	ILE		101	83.760	73.768	10.636	1.00 24.86	E
ATOM	5230	CD1	ILE		101	82.584	74.635	10.197	1.00 25.22	E
ATOM	5231	C	ILE		101	87.538	74.372	11.116	1.00 26.66	E
ATOM	5232	0	ILE			87.859	75.065	12.074	1.00 26.18	E
ATOM	5233	N	SER		102	88.287	74.262	10.029	1.00 31.17	E
ATOM	5234	CA	SER	E	102	89.547	74.977	9.902	1.00 35.36	E
MOTA	5235	CB	SER	E	102	90.619	74.306	10.755	1.00 34.20	E
ATOM	5236	OG	SER	E	102	90.777	72.953	10.374	1.00 40.09	E
MOTA	5237	C	SER	E	102	89.976	74.979	8.448	1.00 36.82	E
MOTA	5238	0	SER	E	102	89.913	73.953	7.777	1.00 36.68	E
MOTA	5239	N	PRO	E	103	90.404	76.139	7.932	1.00 39.96	E
MOTA	5240	CD	PRO		103	90.458	77.473	8.553	1.00 40.07	E
ATOM	5241	CA	PRO		103	90.831	76.190	6.532	1.00 42.01	E
ATOM	5242	CB	PRO		103	90.856	77.682	6.237	1.00 41.76	E
ATOM	5243	CG	PRO		103	91.282	78.258	7.556	1.00 42.86	E
ATOM	5244	C	PRO		103	92.196	75.534	6.390	1.00 44.62	E
ATOM	5245	0	PRO		103	92.943	75.430	7.365	1.00 44.53	E
ATOM	5246	N	SER		104	92.514	75.086	5.181	1.00 47.92	E E
MOTA	5247 5240	CA	SER		104	93.789	74.426	4.920	1.00 50.83	E
ATOM	5248 5240	CB	SER		104	93.712	73.637	3.612	1.00 52.33	E
ATOM	5249	QG	SER	II.	エハギ	94.904	72.901	3.396	1.00 55.60	Ľ

ATOM	5250	С	SER	E 104	94.941	75.422	4.845	1.00 52.18	E
ATOM	5251	0	SER		96.080	75.093	5.186	-	E
ATOM	5252	N	ASN		90.669	78.112		· -	E
ATOM	5253	CA	ASN		90.651	77.795		1.00 47.57	E
ATOM	5254	CB	ASN	· ·	89.863	78.854	0.496		E
ATOM	5255	CG	ASN		90.504	80.219	0.417		
ATOM	5256	ODI		E 113	90.693	80.765	-0.670		E
ATOM	5257	ND2		E 113	90.845	80.781		1.00 55.11	E
ATOM	5258	C	ASN	E 113	90.045		1.572	1.00 55.09	E
MOTA	5259	Ö	ASN	E 113		76.424	-0.001	1.00 44.87	E
ATOM	5260	N	LEU	E 114	89.374	75.852	-0.860	1.00 44.99	E
ATOM	5261	CA	LEU		90.282	75.904	1.197	1.00 41.65	E
ATOM	5261				89.765	74.592	1.568	1.00 38.53	E
ATOM		CB	LEU	E 114	90.823	73.521	1.287	1.00 38.84	E
ATOM	5263	CG		E 114	90.383	72.060	1.441	1.00 40.32	E
	5264	CD1		E 114	89.314	71.726	0.400	1.00 39.94	E
ATOM	5265	CD2		E 114	91.586	71.145	1.266	1.00 40.52	${f E}$
ATOM	5266	C		E 114	89.349	74.523	3.036	1.00 34.78	\mathbf{E}
ATOM	5267	0	LEU		90.173	74.684	3.929	1.00 33.51	E
ATOM	5268	N	LEU		88.063	74.293	3.278	1.00 32.05	E
ATOM	5269	CA	LEU		87.550	74.181	4.641	1.00 29.68	E
ATOM	5270	CB		E 115	86.158	74.809	4.754	1.00 29.84	E
ATOM	5271	CG		E 115	86.046	76.257	5.241	1.00 31.52	E
ATOM	5272	CD1	LEU	E 115	87.101	77.140	4.574	1.00 32.51	E
ATOM	5273	CD2	LEU	E 115	84.636	76.762	4.948	1.00 30.75	E
ATOM	5274	C	LEU	E 115	87.472	72.712	5.034	1.00 27.57	E
MOTA	5275	0	LEU	E 115	86.871	71.900	4.331	1.00 25.33	E
ATOM	5276	N	VAL	E 116	88.089	72.381	6.161	1.00 26.32	E
MOTA	5277	CA	VAL	E 116	88.099	71.014	6.651	1.00 24.42	E
ATOM	5278	CB	VAL	E 116	89.513	70.572	7.075	1.00 24.51	E
ATOM	5279	CG1	VAL	E 116	89.467	69.160	7.641	1.00 22.66	E
MOTA	5280	CG2	VAL	E 116	90.458	70.643	5.879	1.00 26.70	E
ATOM	5281	C	VAL	E 116	87.195	70.842	7.846	1.00 22.77	E
MOTA	5282	0	VAL	E 116	87.376	71.496	8.868	1.00 23.04	E
MOTA	5283	N	CYS	E 117	86.208	69.968	7.717	1.00 22.34	E
ATOM	5284	CA	CYS	E 117	85.326	69.711	8.840	1.00 21.65	E
ATOM	5285	C	CYS	E 117	85.769	68.391	9.466	1.00 19.44	E
ATOM	5286	0	CYS	E 117	85.607	67.319	8.877	1.00 18.95	E
ATOM	5287	CB	CYS	E 117	83.863	69.626	8.401	1.00 22.57	E
ATOM	5288	SG	CYS	E 117	82.771	69.420	9.844	1.00 25.79	E
ATOM	5289	N	SER	E 118	86.355	68.488	10.654	1.00 19.92	E
ATOM	5290	CA	SER	E 118	86.837	67.330	11.387	1.00 17.98	E
ATOM	5291	CB	SER	E 118	88.115	67.671	12.146	1.00 18.33	E
ATOM	5292	OG		E 118	89.121	68.117	11.260	1.00 24.58	E
MOTA	5293	C		E 118	85.798	66.860	12.377	1.00 17.01	E
ATOM	5294	O		E 118	85.507	67.543	13.354	1.00 16.69	E
ATOM	5295	N		0 E 119	85.240	65.688	12.112	1.00 16.58	E
ATOM	5296	CA		E 119	84.242	65.095	12.985	1.00 16.03	E
ATOM	5297	СВ		E 119	83.040	64.582	12.160	1.00 15.47	E
ATOM	5298	CG1		 E 119	81.918	64.147	13.077	1.00 13.47	E
ATOM	5299	CG2	VAL		82.559	65.686	11.216	1.00 10.95	e E
ATOM	5300	C		E 119	85.018	63.960	13.638		
ATOM	5301	0		E 119	85.238	62.906		1.00 17.51 1.00 19.30	E
ATOM	5302	N		E 120	85.442	64.203	13.042		E
ATOM	5303	CA	THR I		86.265		14.871	1.00 18.44	E
ATOM	5304	CB	THR 1		87.562	63.266	15.616	1.00 18.41	E
ATOM	5305	OG1	THR I		87.242	63.962	16.042	1.00 18.11	E
ATOM	5306	CG2	THR 1			65.078	16.887	1.00 17.18	E
ATOM					88.304	64.481	14.835	1.00 16.77	E
ATOM ATOM	5307	C	THR I		85.655	62.656	16.875	1.00 20.11	E
	5308	0		E 120	84.665	63.148	17.417	1.00 21.96	. E
ATOM	5309	N		E 121	86.272	61.566	17.319	1.00 19.96	E
ATOM	5310	CA		E 121	85.882	60.864	18.529	1.00 21.06	E
ATOM	5311	CB		E 121	86.313	61.686	19.745	1.00 25.93	E
ATOM	5312	CG		E 121	87.814	61.765	19.882	1.00 30.02	E
ATOM	5313	OD1		E 121	88.291	62.524	20.756	1.00 34.97	${f E}$
ATOM	5314	OD2		3 121	88.513	61.063	19.114	1.00 31.15	E
ATOM	5315	C		3 121	84.431	60.463	18.709	1.00 20.39	E
ATOM	5316	0		E 121	83.857	60.698	19.766	1.00 22.05	E
ATOM	5317	N		E 122	83.827	59.841	17.708	1.00 19.69	E
ATOM	5318	CA		E 122	82.443	59.429	17.873	1.00 18.28	E
ATOM	5319	CB		E 122	81.538	60.108	16.843	1.00 16.99	E
ATOM	5320	CG		3 122	81.905	59.821	15.417	1.00 16.67	E
ATOM	5321	CD1		E 122	82.770	60.661	14.725	1.00 16.72	E
ATOM	5322			E 122	81.370	58.717	14.756	1.00 17.17	E
ATOM	5323	CE1	PHE E	E 122	83.096	60.410	13.384	1.00 17.00	E

ATOM	5324	CE2	PHE	E	122	81.686	58.456	13.419	1.00	16.82	${f E}$
ATOM	5325	CZ	PHE	E	122	82.549	59.305	12.733	1.00	15.81	E
MOTA	5326	C	PHE	\mathbf{E}	122	82.287	57.925	17.774	1.00	18.35	${f E}$
ATOM	5327	0	PHE	E	122	83.168	57.231	17.272	1.00	15.90	E
ATOM	5328	N	TYR	E	123	81.157	57.436	18.276	1.00	19.49	${f E}$
ATOM	5329	CA	TYR	E	123	80.818	56.021	18.243	1.00	20.92	E
									-		
ATOM	5330	CB	TYR	E	123	81.523	55.261	19.374	1.00	21.02	E
MOTA	5331	CG	TYR	E	123	81.387	53.762	19.247	1.00	20.05	E
ATOM	5332	CD1	TYR	E	123	80.242	53.103	19.688	1.00	21.66	E
MOTA	5333	CE1	TYR	\mathbf{E}	123	80.095	51.726	19.516	1.00	21.85	E
ATOM	5334	CD2	TYR	E	123	82.383	53.009	18.633	1.00	20.08	E
ATOM	5335	CE2	TYR	\mathbf{E}	123	82.250	51.643	18.455	1.00	19.20	E
ATOM	5336	CZ	TYR	E	123	81.105	51.002	18.896	1.00	22.24	E
ATOM	5337	OH	TYR	E	123	80.970	49.640	18.712	1.00	25.26	E
ATOM	5338	C	TYR	E	123	79.311	55.957	18.440	1.00	21.42	E
MOTA	5339	0	TYR	E	123	78.778	56.647	19.305	1.00	23.90	E
ATOM	5340	N	PRO	E	124	78.609	55.100	17.676	1.00	20.39	E
			-								
ATOM	5341	CD	PRO	E	124	77.155	54.937	17.844	1.00	21.24	E
MOTA	5342	CA	PRO	\mathbf{E}	124	79.113	54.177	16.655	1.00	21.61	E
ATOM	5343	CB	PRO	E	1.24	77.956	53.188	16.500	1.00	19.35	${f E}$
ATOM	5344	CG	PRO	\mathbf{E}	124	76.776	54.056	16.670	1.00	19.34	E
MOTA	5345	C	PRO	E	124	79.549	54.802	15.325	1.00	20.84	E
ATOM	5346	0	PRO	E	124	79.602	56.024	15.184	1.00	22.13	${f E}$
ATOM	5347	N	ALA	\mathbf{E}	125	79.862	53.940	14.361	1.00	22.61	E
MOTA	5348	CA	ALA	H	125	80.329	54.341	13.027	1.00	25.48	E
ATOM	5349	CB	ALA	\mathbf{E}	125	80.860	53.121	12.288	1.00	26.06	${f E}$
						79.311	55.058	12.137	1.00	27.38	E
ATOM	5350	C	ALA		125						
MOTA	5351	0	ALA	\mathbf{E}	125	79.681	55.906	11.332	1.00	29.08	E
ATOM	5352	N	GLN	E	126	78.039	54.706	12.268	1.00	29.18	E
ATOM	5353	CA	GLN	E	126	76.990	55.312	11.455	1.00	29.94	E
ATOM	5354	CB	GLN	E	126	75.625	54.737	11.848	1.00	33.48	E
MOTA	5355	CG	GLN	E	126	75.536	53.200	11.840	1.00	39.27	E
ATOM	5356	CD	GLN	E	126	76.067	52.537	13.117	1.00	41.92	E
											E
ATOM	5357	OE1	GLN	E	126	77.271	52.523	13.379	1.00	44.02	
ATOM	5358	NE2	GLN	\mathbf{E}	126	75.159	51.981	13.913	1.00	43.83	E
ATOM	5359	C	GLN	E	126	76.977	56.829	11.621	1.00	28.88	E
ATOM	5360	0	${ t GLN}$	E	126	76.739	57.331	12.719	1.00	28.83	E
ATOM	5361	N	ILE	E	127	77.221	57.558	10.532	1.00	27.90	E
ATOM	5362	CA	ILE	E	127	77.245	59.018	10.591	1.00	25.67	E
ATOM	5363	CB	ILE	\mathbf{E}	127	78.611	59.514	11.150	1.00	25.23	E
								10.084	1.00	21.16	E
MOTA	5364	CG2	ILE	E	127	79.693	59.398				
ATOM	5365	CG1	ILE	E	127	78.504	60.965	11.610	1.00	22.40	E
ATOM	5366	CD1	ILE	E	127	79.610	61.376	12.546	1.00	25.35	E
MOTA	5367	C	ILE	E	127	76.985	59.673	9.230	1.00	26.38	E
ATOM	5368	0	ILE	E	127	77.196	59.065	8.182	1.00	26.20	E
									•		
ATOM	5369	N	LYS	E	128	76.521	60.916	9.252	1.00	25.64	E
MOTA	5370	CA	LYS	\mathbf{E}	128	76.248	61.635	8.016	1.00	29.02	E
			LYS		1.28	74.754	61.566	7.671	1.00	29.97	E
ATOM	5371	CB	,	E							
ATOM	5372	CG	LYS	E	128	74.408	62.178	6.317	1.00	35.17	${f E}$
MOTA	5373	CD	LYS	E	128	75.175	61.487	5.183	1.00	39.63	E
ATOM	5374	CE	LYS	H	128	74,936	62.163	3.836	1.00	41.20	E
ATOM	5375	NZ	LYS	E	128	75,685	61.492	2.731	1.00	44.74	E
			T 370			76.683	63.090		7 00	28.40	E
MOTA	5376	C		E	128			8.154		-	
ATOM	5377	0	LYS	\mathbf{E}	128	76.203	63.812	9.028	7.00	27.15	E
ATOM	5378	N	VAL	E	129	77.600	63.506	7.287	1.00	28.99	E
ATOM	5379	CA	VAL	E	129	78.119	64.866	7.304		29.32	E
ATOM	5380	CB	VAL	\mathbf{E}	129	79.651	64.860	7.502	1.00	30.69	E
					129	80.171	66.282	7.654		27.54	E
ATOM	5381	CG1	VAL								
ATOM	5382	CG2	VAL	E	129	80.014	64.012	8.721	1.00	30.82	E
ATOM	5383	С	VAL	H.	129	77.788	65.574	5.992	1 00	30.45	E
ATOM	5384	0	VAL	E	129	78.042	65.039	4.915		30.36	E
ATOM	5385	N	ARG	E	130	77.221	66.775	6.090	1.00	31.17	E
ATOM	5386	CA	ARG	E	130	76.851	67.562	4.914		32.17	E
ATOM	5387	CB	ARG	\mathbf{E}	130	75.330	67.626	4.764	1.00	34.73	E
										40.85	E
ATOM	5388	CG	ARG			74.632	66.335	4.400			
ATOM	5389	CD	ARG	E	130	73.121	66.527	4.511	1.00	46.16	E
ATOM	5390	NE	ARG	E		72.365	65.456	3.864	7 00	51.33	E
MOTA	5391	CZ	ARG	E	130	71.046	65.308	3.959	1.00	53.45	E
ATOM	5392	NHI	ARG	\mathbf{E}	130	70.327	66.162	4.680	1.00	54.21	E
										53.97	
ATOM	5393	NH2	ARG	E	130	70.444	64.307	3.329			E
ATOM	5394	C	ARG	E	130	77.359	68.994	5.017	1.00	30.88	E
			ARG	E		77.321	69.590	6.093	1.00		E
MOTA	5395	0									
MOTA	5396	N	TRP	E	131	77.831	69.542	3.900		29.14	E
ATOM	5397	CA.	TRP	E	131	78.291	70.928	3.865	1.00	29.57	E
	·			-			<u>-</u>			-	_

ATOM	5398	B CB TRP E 131	70 F2	. =			
ATOM			79.53			5 1.00 27.97	E
			80.80	9 70.979	3.760	1.00 29.37	E
ATOM			81.342	2 71.949	4.671	L 1.00 29.95	E
ATOM		L CE2 TRP E 131	82.55	l 71.427	5.174	- -	E
ATOM	5402	CE3 TRP E 131	80.913				
ATOM	5403	CD1 TRP E 131	81.689	-			E
ATOM	5404		82.738		• • •	_,,,,	E
ATOM							E
ATOM			83.340	·	6.095	1.00 28.79	E
			81.697		6.027	1.00 31.30	E
ATOM	Ī		82.900	73.350	6.509	1.00 31.69	E
ATOM	5408	C TRP E 131	77.185	71.817	3.301		E
ATOM	5409	O TRP E 131	76.449	71.413	2.392		
ATOM	5410	N PHE E 132	77.081		3.842		E
ATOM	5411		76.078	· - ·			E
ATOM	5412				3.405		E
ATOM	5413		74.963		4.443	1.00 32.09	E
ATOM			74.041	· - -	4.461	1.00 33.03	E
	5414		72.913	72.896	3.650	1.00 35.25	E
ATOM	5415	CD2 PHE E 132	74.306	71.822	5.273		E
MOTA	5416	CE1 PHE E 132	72.055	71.794	3.646		E
ATOM	5417	CE2 PHE E 132	73.460		5.279		
ATOM	5418	CZ PHE E 132	72.330				E
ATOM	5419	C PHE E 132	76.668	-	4.461	1.00 35.97	E
ATOM	5420				3.182	1.00 32.06	E
ATOM	5421		77.537		3.929	1.00 29.15	E
		N ARG E 133	76.186	76.026	2.138	1.00 34.68	E
ATOM	5422	CA ARG E 133	76.613	77.375	1.809	1.00 37.78	E
ATOM	5423	CB ARG E 133	77.281	77.420	0.434	1.00 40.14	E
ATOM	5424	CG ARG E 133	77.755	78.810	0.005		E
MOTA	5425	CD ARG E 133	78.474		-1.341		
ATOM	5426	NE ARG E 133	79.096				E
ATOM	5427	CZ ARG E 133			-1.738		E
ATOM	5428		78.441		-2.226		E
			77.124		-2.387	1.00 51.33	E
ATOM	5429	NH2 ARG E 133	79.111		-2.562	1.00 52.46	E
ATOM	5430	C ARG E 133	75.343	78.204	1.792	1.00 38.70	E
ATOM	5431	O ARG E 133	74.569	78.154	0.835	1.00 38.81	E
ATOM	5432	N ASN E 134	75.119	78.940	2.872		E
ATOM	5433	CA ASN E 134	73.941		2.984		
ATOM	5434	CB ASN E 134	74.040			1.00 42.21	E
ATOM	5435	CG ASN E 134		80.952	1.988	· · ·	E
ATOM	5436		75.383			1.00 39.50	E
		OD1 ASN E 134	75.796	82.151	3.104	1.00 35.36	E
ATOM	5437	ND2 ASN E 134	76.071	81.733	0.917	1.00 39.94	E
ATOM	5438	C ASN E 134	72.652	79.000	2.734	1.00 43.61	E
MOTA	5439	O ASN E 134	71.899	79.306	1.809	1.00 45.62	E
ATOM	5440	N ASP E 135	72.403	77.983	3.550	1.00 45.40	
ATOM	5441	CA ASP E 135	71.189	77.178			E
ATOM	5442	C ASP E 135			3.413	1.00 47.16	E
ATOM	5443		71.147	76.279	2.173	1.00 48.15	\mathbf{E}
			70.205	75.504	1.996	1.00 49.25	E
ATOM	5444	N GLN E 136	72.158	76.387	1.316	1.00 48.16	E
ATOM	5445	CA GLN E 136	72.226	75.561	0.113	1.00 47.50	E
ATOM	5446	C GLN E 136	73.254	74.445	0.313	1.00 47.38	Ē
MOTA	5447	O GLN E 136	74.418	74.711	0.627	1.00 46.25	E
MOTA	5448	N GLU E 137	72.829	73.197	0.139		
ATOM	5449	CA GLU E 137	73.749			1.00 47.09	E
ATOM	5450	CB GLU E 137		72.079	0.308	1.00 47.41	E
ATOM	5451		72.992	70.752	0.406	1.00 47.53	${f E}$
			73.921	69.570	0.653	1.00 49.67	E
ATOM	5452	CD GLU E 137	73.210	68.334	1.166	1.00 51.28	E
ATOM	5453	OE1 GLU E 137	73.911	67.336	1.432	1.00 52.31	E
ATOM	5454	OE2 GLU E 137	71.965	68.352	1.306	1.00 51.54	E
MOTA	5455	C GLU E 137	74.755	72.016	-0.833	1.00 47.37	
ATOM	5456	O GLU E 137	74.397	72.163			E
ATOM		N GLU E 138		<u></u>	-2.000	1.00 47.51	E
ATOM	5458	CA GLU E 138	76.018		-0.477	1.00 47.53	E
			77.104		-1.444	1.00 48.48	E
ATOM	5459	CB GLU E 138	78.266	72.617	-1.011	1.00 49.89	E
ATOM	5460	CG GLU E 138	77.949	74.096	-0.973	1.00 54.83	E
ATOM	5461	CD GLU E 138	77.911	74.720	-2.354	1.00 57.91	E
ATOM	5462	OE1 GLU E 138	78.953		-3.044	1.00 59.04	E
ATOM	5463	OE2 GLU E 138	76.846		-2.748		
ATOM		C GLU E 138	77.593			1.00 58.96	E
ATOM		O GLU E 138			-1.532	1.00 48.42	E
ATOM			77.898		-0.513	1.00 48.62	E
		N THR E 139	77.665	69.754	-2.748	1.00 47.87	E
ATOM		CA THR E 139	78.135	68.387	-2.959	1.00 48.16	E
MOTA		CB THR E 139	77.027	67.498	-3.556	1.00 49.05	E
ATOM	5469	OG1 THR E 139	76.464		-4.710	1.00 51.25	E
MOTA	5470	CG2 THR E 139	75.938		-2.525	1.00 48.03	
ATOM		C THR E 139	79.339				E
					-3.895	1.00 46.96	E

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ATOM	5472	. 0	THR E 139	80.2	45 6	7.574	-3.779	7 00	46.46	E
ATOM	5473	N	ALA E 140			9.346			46.59	
ATOM	5474	CA				9.488				E
ATOM	5475				_				45.07	E
ATOM	5476		ALA E 140			0.244		· · · -	44.64	E
						0.276		1.00	43.57	E
ATOM	5477		ALA E 140		24 7	1.293	-4.386	1.00	43.33	E
ATOM	5478	N	GLY E 141	82.7	56 6:	9.805	-5.091	1.00	41.31	E
ATOM	5479	CA	GLY E 141	83.8	33 7	0.485	-4.398	1.00	38.27	E
ATOM	5480	C	GLY E 141	84.0	53 6	9.854			36.91	E
ATOM	5481	0	GLY E 141			0.264				
ATOM	5482	N	VAL E 142	. – • -	_	8.849		_	37.78	E
ATOM	5483	CA							33.36	E
ATOM						8.164			32.16	E
	5484					7.844	-0.847	1.00	31.40	E
ATOM	5485	CG			40 66	5.995	0.407	1.00	28.96	E
MOTA	5486	CG	2 VAL E 142	81.2	45 69	9.134	-0.516	1.00	33.20	E
ATOM	5487	C	VAL E 142	84.1	40 66	5.859	-1.576		31.49	E
MOTA	5488	0	VAL E 142	83.8	52 66	5.032	-2.450		31.67	E
ATOM	5489	N	VAL E 143	85.1		5.684	-0.696			
ATOM	5490	CA		85.9					30.51	E
ATOM	5491	CB				5.473	-0.675		30.35	E
ATOM			· – – 	87.36		5.731	-1.161	1.00	30.33	E
	5492	CG		88.09		1.408	-1.348	1.00	32.44	E
ATOM	5493	CG:	-	87.34	£7 66	5.503	-2.460	1.00	33.96	E
ATOM	5494	C	VAL E 143	85.96	66 64	.973	0.767	1.00	29.68	E
ATOM	5495	0	VAL E 143	86.24	2 65	.733	1.695		29.63	E
ATOM	5496	N	SER E 144	85.69		.689	0.946		28.32	
ATOM	5497	CA	SER E 144	85.70		.090	2.268			E
ATOM	5498	CB	SER E 144	84.29					25.38	E
ATOM	5499	OG				.613	2.622		26.70	E
				84.30		845	3.807	1.00	28.37	E
ATOM	5500	C	SER E 144	86.66		916	2.361	1.00	24.56	王
ATOM	5501	0	SER E 144	86.82	4 61	148	1.412	1.00	23.42	E
MOTA	5502	N	THR E 145	87.32	0 61	.790	3.506	1.00	24.40	E
ATOM	5503	CA	THR E 145	88.21	.8 60	.666	3.726		24.38	E
ATOM	5504	CB	THR E 145	89.10	3 60	.849	4.983		24.55	E
ATOM	5505	OG		88.27		.815	6.155			
ATOM	5506	CG2	• • • • • •						21.59	E
ATOM	5507	C		89.85		.162	4.935		24.64	E
			THR E 145	87.25		.539	4.055	1.00	23.78	E
ATOM	5508	0	THR E 145	86.06		.766	4.242	1.00	23.97	E
ATOM	5509	N	PRO E 146	87.74	5 58	.300	4.099	1.00	25.25	${f E}$
ATOM	5510	CD	PRO E 146	88.99	3 57	.713	3.585		25.42	E
ATOM	5511	CA	PRO E 146	86.77		.264	4.447		25.00	E
ATOM	5512	CB	PRO E 146	87.43		.983	3.951		26.60	
ATOM	5513	CG	PRO E 146	88.90						E
ATOM	5514	C	PRO E 146			.293	4.094		27.24	E
ATOM				86.59	_	.284	5.976		23.26	E
	5515	0	PRO E 146	87.28		.030	6.672	1.00	21.73	E
ATOM	5516	N	LEU E 147	85.66	9 56	.492	6.495	1.00	23.85	E
ATOM	5517	CA	LEU E 147	85.47	6 56	.419	7.936	1.00	23.63	E
ATOM	5518	CB	LEU E 147	84.35	5 55	.428	8.260		25.11	E
ATOM	5519	CG	LEU E 147	83.97		.241	9.731		28.28	E
ATOM	5520	CD1	LEU E 147	83.39		.530	10.270			
ATOM	5521		LEU E 147	82.96				1.00		E
ATOM	5522	C				.116	9.867	1.00		E
			LEU E 147	86.81		.915	8.503	1.00		${f E}$
ATOM	5523	0	LEU E 147	87.36		.944	8.003	1.00	23.04	E
ATOM	5524	N	ILE E 148	87.33	7 56	.574	9.530	1.00	21.06	E
MOTA	5525	$\mathbf{C}\mathbf{A}$	ILE E 148	88.61	4 56.	.156	10.102	1.00	19.40	E
ATOM	5526	CB	ILE E 148	89.588	3 57.	.355	10.200	1.00 :		E
ATOM	5527	CG2	ILE E 148	90.90		.922	10.835	1.00		
ATOM	5528	CG1		89.854		918	8.803			E
ATOM	5529	CD1	ILE E 148					1.00		E
ATOM	5530			90.594	_	.225	8.821	1.00		\mathbf{E}
		C	ILE E 148	88.449		534	11.489	1.00	17.19 .	E
ATOM	5531	0	ILE E 148	87.820	56.	.118	12.360	1.00	15.81	E
ATOM	5532	N	ARG E 149	89.019	54.	344	11.677	1.00	15.23	E
ATOM	5533	CA	ARG E 149	88.948	3 53.	638	12.956	1.00	16.42	E
ATOM	5534	CB	ARG E 149	88.906	52.	128	12.724	1.00 2		E
ATOM	5535	CG	ARG E 149	88.903	_	289	14.000	1.00 2		
ATOM	5536	CD	ARG E 149	88.963	_					E
ATOM	5537	NE				802	13.649	1.00 2		E
			ARG E 149	87.825		382	12.830	1.00 2		E
ATOM	5538	CZ	ARG E 149	86.623		084	13.313	1.00 2	22.89	E
ATOM	5539	NH1	ARG E 149	85.650	48.	718	12.490	1.00 2	24.25	E
ATOM	5540	NH2	ARG E 149	86.398	49.	139	14.619	1.00 2		E
MOTA	5541	C	ARG E 149	90.174		983	13.786	1.00		E
ATOM	5542	0	ARG E 149	91.305			13.363			
ATOM	5543	N	ASN E 150					1.00 1		E
ATOM	5544	CA		89.953		558	14.963	1.00 1		E
				91.061			15.825	1.00 1		E
ATOM	5545	CB	ASN E 150	90.662	56.	125	16.740	1.00 1	.3.37	E

3 more		aa	3 C) T	T-1	150	00 070	F7 303	15.955	1 00	15.55	E
ATOM	5546	CG	NZA			90.278	57.383		•		
ATOM	5547	OD1	ASN	E	150	90.922	57.739	14.955	1.00	14.20	E
MOTA	5548	ND2	ASN	E	150	89.233	58.068	16.414	1.00	15.61	E
MOTA	5549	С	ASN	E	150	91.576	53.786	16.670	1.00	16.79	${f E}$
ATOM	5550	0			150	92.694	53.838	17.180	1.00	18.80	E
									1.00	16.63	E
ATOM	5551	N		E	151	90.764	52.745	16.813			
MOTA	5552	CA	GLY	E	151	91.164	51.587	17.593	1.00	18.68	E
ATOM	5553	С	GLY	E	151	90.879	51.684	19.080	1.00	20.19	E
ATOM	5554	0	GLY	E	151	91.087	50.725	19.818	1.00	21.39	E
			-	E	152	90.409	52.836	19.539	1.00	19.57	E
MOTA	5555	N									
MOTA	5556	CA	ASP	E	152	90.108	52.986	20.954	1.00	19.09	E
ATOM	5557	CB	ASP	E	152	90.865	54.177	21.531	1.00	18.53	E
MOTA	5558	CG	ASP	E	152	90.498	55.481	20.856	1.00	21.27	E
ATOM	5559	OD1	ASP	E	152	89.736	55.453	19.864	1.00	20.11	E
							56.531	21.321	1.00	22.57	E
ATOM	5560	OD2		E	152	90.984	_				
MOTA	5561	C	ASP	E	152	88.605	53.156	21.182	1.00	19.23	E
ATOM	5562	0	ASP	E	152	88.177	53.840	22.113	1.00	17.78	E
ATOM	5563	N	TRP	E	153	87.816	52.522	20.318	1.00	18.88	E
ATOM	5564	CA		E	153	86.356	52.566	20.391	1.00	18.61	E
						85.862	52.162	21.788	1.00	17.06	E
MOTA	5565	CB		E	153						
ATOM	5566	CG	TRP	\mathbf{E}	153	86.084	50.690	22.085	1.00	17.90	E
ATOM	5567	CD2	TRP	E	153	85.165	49.612	21.830	1.00	18.84	\mathbf{E}
ATOM	5568	CE2	TRP	E	153	85.804	48.414	22.222	1.00	16.88	E
ATOM	5569	CE3		E	153	83.862	49.544	21.308	1.00	18.29	E
				-			50.114	22.604	1.00	16.70	E
MOTA	5570	CD1		E	153	87.209					
ATOM	5571	NEI	TRP	E	153	87.049	48.747	22.688		17.49	E
MOTA	5572	CZ2	TRP	\mathbf{E}	153	85.189	47.164	22.109	1.00	16.54	E
ATOM	5573	CZ3	TRP	E	153	83.250	48.303	21.196	1.00	17.19	E
		CH2		E	153	83.917	47.129	21.597	1.00	17.24	E
MOTA	5574									18.97	E
ATOM	5575	C		E	153	85.732	53.887	19.975	1.00		
ATOM	5576	0	TRP	E	153	84.696	54.300	20.508	1.00		E
MOTA	5577	N	THR	\mathbf{E}	154	86.378	54.546	19.016	1.00	19.20	E
ATOM	5578	CA	THR	E	154	85.876	55.794	18,444	1.00	19.92	E
	5579	CB	THR		154	86.442		19.129	1.00	21.42	E
ATOM								18.958		19.26	E
MOTA	5580	OG1	THR		154	87.865					
MOTA	5581	CG2	THR	E	154	86.085	57.096	20.599	1.00		E
ATOM	5582	C	THR	E	154	86.314	55.835	16.992	1.00	18.66	E
MOTA	5583	O	THR	E	154	87.270	55.156	16.603	1.00	19.45	E
ATOM	5584	N	PHE	E	155	85.609		16.193	1.00	18.54	臣
										19.04	E
ATOM	5585	CA	PHE	E	155	85.940		14.779			
MOTA	5586	CB	PHE	E	155	84.821	56.252	13.882		20.71	E
ATOM	5587	CG	PHE	E	155	84.524	54.794	14.060	1.00	23.03	E
ATOM	5588	CD1	PHE	E	155	83.492	54.375	14.898	1.00	23.94	E
ATOM	5589	CD2		E		85.255		13.365	1.00	23.32	E
								15.037		23.82	E
ATOM	5590	CE1			1.55	83.189					
ATOM	5591	CE2	PHE	E	155	84.962	52.476	13.497		24.46	E
MOTA	5592	CZ	PHE	E	155	83.930	52.068	14.333	1.00	24.51	E
ATOM	5593	C	PHE	E	155	86.109	58.265	14.459	1.00	19.30	E
ATOM	5594	Ō	PHE	E		85.791	59.134	15.275	1.00	19.12	E
						86.613		13.265		17.46	E
ATOM	5595	N	GLN								E
MOTA	5596	CA	GLN	E	156	86.748		12.824		17.87	
ATOM	5597	CB	GLN	E	156	88.081	60.546	13.264	1.00	19.74	臣
ATOM	5598	CG	GLN	E	156	89.330	59.948	12.640	1.00	19.80	E
ATOM	5599	CD	GLN	E	156	90.551	60.785	12.950	1.00	21.46	\mathbf{E}
ATOM	5600	OE1				90.660		12.503		21.30	E
								13.734		21.38	E
MOTA	5601	NE2		E		91.469					
MOTA	5602	C	GLN	E	156	86.629	59.989	11.316	1.00		E
ATOM	5603	0	GLN	E	156	86.85 <i>6</i>	58.999	10.616	1.00	17.25	E
MOTA	5604	N	ILE	E	157	86.252	61.159	10.823	1.00	17.46	E
MOTA	5605	CA			157	86.128		9.397	1.00	18.92	E
								8.898	1.00		E
MOTA	5606	CB			157	84.746					
ATOM	5607	CG2	ILE	E	157	83.659		9.545	1.00		E
MOTA	5608	CG1	. ILE	E	157	84.704	60.994	7.369	1.00	21.06	E
ATOM	5609	CDI				83.541	60.218	6.756	1.00	22.57	E
MOTA	5610	C	ILE			86.349		9.083		20.28	E
								9.808		20.70	E
MOTA	5611	0	ILE			85.887					
ATOM	5612	N	LEU	E	158	87.094		8.019		21.79	E
MOTA	5613	CA	LEU	E	158	87.363	64.470	7.601		23.40	E
MOTA	5614	CB	LEU	E	158	88.869	64.706	7.466	1.00	25.42	\mathbf{E}
ATOM	5615	CG	LEU			89.621		8.731	1.00	29.38	E
						89.384		9.864		27.98	E
MOTA	5616	CD1	_								E
ATOM	5617		E LEU			91.118		8.412		30.79	
MOTA	5618	C	LEU	E	158	86.664	64.738	6.271		23.62	E
ATOM	5619	0	LEU	F	158	86.938	64.081	5.264	1.00	22.86	E
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ATOM	5620	N	VAL E		85.747	65.702	6.290	1.00 22.98	E
ATOM	5621	CA.	VAL E		84.990	66.087	5.112 5.417	1.00 21.37 1.00 20.53	E E
MOTA	5622	CB		159	83.476 82.684	66.104 66.407	5.417 4.149	1.00 20.53	E
ATOM ATOM	5623 5624	CG1 CG2	VAL E		83.058	64.756	6.002	1.00 15.86	E
ATOM	5625	C		159	85.468	67.469	4.710	1.00 22.21	E
MOTA	5626	0		159	85.253	68.444	5.423	1.00 22.87	E
ATOM	5627	N	MET E	160	86.116	67.539	3.555	1.00 25.37	E
ATOM	5628	CA	MET E	160	86.681	68.779	3.049	1.00 27.07	E
MOTA	5629	CB	MET E	160	88.088	68.494	2.533	1.00 29.57 1.00 35.17	E E
ATOM	5630	CG		160 160	88.996 90.519	67.954 67.185	3.633 3.065	1.00 35.17	E
ATOM ATOM	5631 5632	SD CE	MET E	160	90.011	65.462	2.985	1.00 40.10	E
ATOM	5633	C	•	160	85.848		1.979	1.00 28.93	E
ATOM	5634	0	MET E	160	85.191	68.817	1.162	1.00 28.47	E
MOTA	5635	N	TEA E	161	85.875	70.793	1.997	1.00 29.41	E
ATOM	5636	CA	LEU E	161	85.123	71.574	1.031	1.00 31.54 1.00 30.26	E E
ATOM	5637	CB		161 161	83.931 83.183	72.258 73.297	1.708 0.860	1.00 30.26 1.00 30.70	E
ATOM ATOM	5638 5639	CG CD1		161	82.515	72.618	-0.332	1.00 29.72	E
ATOM	5640	CD2		161	82.145	74.020	1.728	1.00 31.55	E
ATOM	5641	C	LEU E	161	85.990	72.625	0.363	1.00 32.10	E
MOTA	5642	0		161	86.575	73.473	1.029	1.00 32.90	E
MOTA	5643	N	GLU E		86.063	72.549	-0.960	1.00 35.11 1.00 38.40	e E
MOTA	5644	CA	GLU E	162 162	86.820 87.191	73.491 72.838	-1.771 -3.105	1.00 38.40	E
MOTA MOTA	5645 5646	CB CG	GLU E	162	87.783	73.776	-4.148	1.00 48.21	E
ATOM	5647	CD		162	89.099	74.381	-3.711	1.00 52.47	E
MOTA	5648	OE1	GLU E	162	90.006	73.611	-3.327	1.00 54.02	E
ATOM	5649	OE2	GLU E	162	89.228	75.627	-3.759	1.00 56.21	E
ATOM	5650	C			85.892	74.673	-2.008	1.00 39.06 1.00 39.27	e E
MOTA	5651	O		162 163	84.750 86.369	74.490 75.884	-2.422 -1.747	1.00 39.27	E
ATOM ATOM	5652 5653	N CA			85.520	77.049	-1.938	1.00 43.18	E
ATOM	5654	CB	MET E		84.546	77.171	-0.761	1.00 45.15	E
ATOM	5655	CG	MET E	163	85.155	76.900	0.612	1.00 47.55	E
MOTA	5656	SD	MET E		86.318	78.152	1.185	1.00 52.18	E
MOTA	5657	CE	MET E		85.186	79.345 78.371	1.941 -2.151	1.00 50.37 1.00 43.77	E E
ATOM ATOM	5658 5659	C O	MET E		86.245 87.458	78.477	-1.953	1.00 41.87	E
MOTA	5660	И	THR E		85.474	79.371	-2.571	1.00 45.83	E
ATOM	5661	CA	THR E		85.981	80.714	-2.827	1.00 49.20	E
MOTA	5662	CB	THR E	164	85.585	81.177	-4.241	1.00 50.11	E
MOTA	5663	OG1			86.036	80.208	-5.199	1.00 49.28 1.00 50.19	E E
ATOM	5664 5665	CG2 C	THR E		86.204 85.371	82.535 81.652	-4.559 -1.785	1.00 50.19	E
ATOM ATOM	5665 5666	0	THR E		84.169	81.916	-1.802	1.00 50.64	E
ATOM	5667	N	PRO E		86.198	82.170	-0.864	1.00 53.75	E
MOTA	5668	CD	PRO E	165	87.667	82.057	-0.818	1.00 54.65	E
ATOM	5669	CA	PRO E	•	85.719	83.072	0.185	1.00 56.16	E E
ATOM	5670	CB	PRO E		86.965 88.057	83.299 83.262	1.036 0.019	1.00 55.47 1.00 55.93	E
ATOM ATOM	5671 5672	CG C	PRO E		85.098	84.381	-0.291	1.00 58.83	E
ATOM	5673	0	PRO E		85.673	85.100	-1.112	1.00 58.35	E
ATOM	5674	N	GLN E	166	83.912	84.666	0.239	1.00 61.77	臣
ATOM	5675	CA	GLN E		83.173	85.885	-0.065	1.00 63.96	E
MOTA	5676	CB	GLN E		82.103	85.616 85.236	-1.123 -2.481	1.00 64.28 1.00 66.42	E E
ATOM ATOM	5677 5678	CG CD	GLN E		82.662 81.643	85.392	-3.596	1.00 67.38	E
MOTA	5679	OE1			81.937	85.124	-4.761	1.00 68.28	E
ATOM	5680	NE2	_		80.437	85.832	-3.244	1.00 66.50	E
MOTA	5681	C	GLN E	166	82.521	86.396	1.223	1.00 65.40	E
MOTA	5682	0	GLN E		81.974	85.614	2.007	1.00 65.65	E E
ATOM	5683	N	ARG E		82.589 82.017	87.707 88.302	1.444 2.647	1.00 65.80 1.00 65.27	E
MOTA MOTA	5684 5685	CA CB	ARG E		82.353	89.795	2.706	1.00 63.27	E
ATOM	5686	CG	ARG E		82.221	90.423	4.095	1.00 70.91	E
ATOM	5687	CD	ARG E		83.216	89.813	5.085	1.00 73.36	E
MOTA	5688	NE	ARG E		83.244	90.532	6.359	1.00 75.19	E
ATOM	5689	CZ	ARG E	-	84.012	90.199	7.394	1.00 75.48 1.00 75.50	E E
MOTA MOTA	5690 5691	NH:			84.824 83.968	89.151 90.916	7.318 8.509	1.00 75.83	E
ATOM ATOM	5691 5692		ARG E		80.504	88.100	2.684	1.00 63.81	E
ATOM	5693	0	ARG E		79.816	88.254	1.672	1.00 62.94	E
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ATOM	5694	N	$G\Gamma \lambda$	Ħ	168	79.991	۶	37.751	3.860	1.00	61.88	E
		CA	GLY		168	78.567		37.519	4.004		58.78	E
ATOM	5695								3.959		57.24	E
ATOM	5696	C	GLY		168	78.243		36.036				
MOTA	5697	0	$\mathbf{G}\mathbf{\Gamma}\mathbf{X}$		168	77.262		35.594	4.558		57.26	E
ATOM	5698	N	ASP	E	169	79.066	8	35.263	3.249		54.67	E
MOTA	5699	CA	ASP	E	169	78.849	8	33.823	3.140	1.00	52.07	E
MOTA	5700	CB	ASP	E	169	79.799	1	83.186	2.116	1.00	52.03	E
ATOM	5701	CG	ASP	E	169	79.329	8	33.359	0.683	1.00	52.57	E
ATOM	5702	OD1	ASP	E	169	78.105	8	83.453	0.457	1.00	51.86	E
MOTA	5703	OD2			169	80.188		83.376	-0.223	1.00	52.34	E
ATOM	5704	C			169	79.027		33.096	4.463		49.54	E
						79.993		33.322	5.196		49.84	E
MOTA	5705	0			169							E
MOTA	5706	N	VAL		170	78.082		32.214	4.758		46.54	
ATOM	5707	CA			170	78.136		81.418	5.970		43.15	E
MOTA	5708	CB	VAI_1	E	170	76.903		81.669	6.871		42.70	E
MOTA	5709	CG1	VAL	E	170	76.997	1	80.819	8.138	1.00	41.36	E
ATOM	5710	CG2	VAL	E	170	76.814		83.146	7.227	1.00	41.14	E
ATOM	5711	C	VAL	E	170	78.172	•	79.948	5.555	1.00	41.66	E
MOTA	5712	0	VAL	E	170	77.216	•	79.432	4.972	1.00	40.25	E
ATOM	5713	N	TYR	E	171	79.289	•	79.287	5.833	1.00	39.16	E
ATOM	5714	CA	TYR		171	79.438	•	77.877	5.502	1.00	38.16	E
ATOM	5715	CB		E	171	80.836		77.617	4.953		38.66	E
		CG	TYR		171	81.035		78.237	3.598	1.00		E
ATOM	5716										38.79	E
MOTA	5717	CD1	TYR		171	80.740		77.522	2.440			
ATOM	5718	CE1				80.852		78.105	1.186		40.42	E
MOTA	5719	CD2	TYR	E	171	81.451		79.561	3.471		38.62	E
ATOM	5720	CE2	TYR	E	171	81.565		80.160	2.219		40.32	E
ATOM	5721	CZ	TYR	E	171	81.262		79.424	1.079	1.00	41.26	E
ATOM	5722	OH	TYR	E	171	81.350		80.004	-0.166	1.00	42.98	E
ATOM	5723	C	TYR	E	171	79.206	•	77.076	6.764	1.00	37.15	E
ATOM	5724	0	TYR	E	171	79.755	. ,	77.398	7.813	1.00	37.94	E
MOTA	5725	N	THR		172	78.384		76.037	6.672	1.00	35.12	E
		CA	THR		172	78.091		75.229	7.842		34.42	E
ATOM	5726					76.654		75.496	8.367		35.21	E
ATOM	5727	CB	THR		172							E
MOTA	5728	OG1			172	76.184		74.351	9.094		35.96	
MOTA	5729	CG2			172	75.706		75.790	7.226		38.35	E
ATOM	5730	C	THR	E	172	78.263		73.734	7.638		32.90	E
MOTA	5731	0	THR	E	172	77.875	;	73.188	6.604	1.00	31.57	E
ATOM	5732	N	CYS	E	173	78.858	}	73.090	8.643	1.00	30.59	E
ATOM	5733	CA	CYS	E	173	79.078	}	71.646	8.640	1.00	29.35	E
MOTA	5734	C	CYS	E	173	77.923	3	71.058	9.454	1.00	29.72	E
ATOM	5735	0	CYS	E	173	77.771		71.337	10.645	1.00	28.89	E
ATOM	5736	CB	CYS	E	173	80.424		71.299	9.287	1.00	27.53	E
ATOM	5737	SG	CYS	E	173	80.875		69.541	9.133	1.00		E
				E	174	77.109		70.251	8.788	1.00		E
ATOM	5738	N	HIS					69.642	9.381		28.54	E
ATOM	5739	CA	HIS	E	174	75.925				1.00		E
MOTA	5740	CB	HIS		174	74.770		69.881	8.399			
ATOM	5741	CG	HIS			73.457		69.311	8.823		30.98	E
ATOM	5742	CD2	HIS	E	174	72.367		69.899	9.369	1.00		E
MOTA	5743	ND1	HIS	E	174	73.124	<u>F</u>	67.988	8.630		31.68	E
ATOM	5744	CE1	HIS	E	174	71.883	3	67.785	9.034	1.00	33.26	E
ATOM	5745	NE2	HIS	E	174	71.401	_	68.929	9.487	1.00	34.66	E
ATOM	5746	С	HIS	E	174	76.173	3	68.151	9.650	1.00	27.83	E
ATOM	5747	0	HIS	E	174	76.438	3	67.375	8.728	1.00	27.35	E
ATOM	5748	N	VAL	E	175	76.085	5	67.753	10.917	1.00	26.27	E
ATOM	5749	CA	VAL			76.349		66.365	11.284	1.00	26.34	E
ATOM	5750	CB			175	77.584		66.281	12.215		23.90	E
						77.807		64.850	12.663		19.67	E
ATOM	5751	CG1				78.818			11.491	1.00		E
ATOM	5752	CG2						66.813				E
MOTA	5753	C	LAV			75.199		65.603	11.938		27.67	
ATOM	5754	0	VAL	E	175	74.587		66.064	12.904		26.77	E
ATOM	5755	N	GLU	E	176	74.917	7	64.423	11.399		29.83	E
MOTA	5756	CA	GLU	E	176	73.864	1	63.564	11.929		32.99	E
ATOM	5757	CB	GLU	E	176	72.842	2	63.231	10.839	1.00	34.86	E
ATOM	5758	CG	GLU	E	176	72.076	ŝ	64.441	10.319	1.00	40.13	E
MOTA	5759	CD			176	71.204		64.107	9.124	1.00	44.38	E
ATOM	5760	OE1			176	70.292		63.265	9.269		46.31	E
		OE2			176	71.433		64.682	8.037		47.49	E
MOTA	5761					74.526		62.289	12.445		32.24	E
MOTA	5762	C			176						32.24	E
ATOM	5763	0			176	75.296		61.646	11.734			E
ATOM	5764	N	HIS		177	74.220		61.934	13.686		31.66	E
MOTA	5765	CA			177	74.803		60.761	14.311		30.50	
ATOM	5766	CB	HIS			76.147		61.161	14.927		29.59	E
ATOM	5767	CG	HIS	E	177	76.871	l	60.034	15.582	1.00	28.23	E
								4	04			

WO	03/030	704							
ATOM	5768	CD2	HIS	E 177	77.752	59.134	15.086	1.00 28.22	E
MOTA	5769	NDl	HIS	E 177	76.679	59.698	16.903	1.00 27.71	E
MOTA	5770		HIS		77.410	58.636	17.194	1.00 29.83	E
MOTA	5771			E 177	78.070	58.274	16.108	1.00 29.78	E
MOTA	5772	C	· -	E 177	73.854	60.195	15.373	1.00 30.09	E
ATOM	5773	0	HIS		73.189	60.942	16.083	1.00 29.91	E
ATOM	5774	N		E 178	73.781	58.862	15.496	1.00 31.45	E
MOTA	5775	CD	PRO		74.485	57.842 58.226	14.697 16.481	1.00 31.00 1.00 31.44	E E
ATOM ATOM	5776 5777	CA CB		E 178 E 178	72.898 73.370	56.779	16.467	1.00 31.44	E
ATOM	5778	CG		E 178	73.704	56.578	15.028	1.00 31.16	E
ATOM	5779	C		E 178	72.896	58.826	17.893	1.00 31.78	E
ATOM	5780	0		E 178	71.903	58.727	18.611	1.00 32.84	E
ATOM	5781	N		E 179	73.996	59.448	18.292	1.00 30.31	E
ATOM	5782	CA	SER	E 179	74.087	60.039	19.624	1.00 30.84	E
MOTA	5783	CB	SER	E 179	75.552	60.155	20.038	1.00 29.11	E
ATOM	5784	OG	SER	E 179	76.240	61.049	19.176	1.00 24.79	E
ATOM	5785	C	SER	E 179	73.452	61.424	19.717	1.00 32.75	E
MOTA	5786	0		E 179	73.330	61.982	20.804	1.00 32.78	E
ATOM	5787	N	LEU		73.046	61.981	18.583	1.00 35.18	E
ATOM	5788	CA		E 180	72.477	63.317	18.578	1.00 37.31	E
MOTA	5789	CB		E 180	73.098 74.610	64.132 64.337	17.448 17.528	1.00 35.77 1.00 36.46	E E
ATOM ATOM	5790 5791	CG	LEU	E 180 E 180	75.097	65.018	16.259	1.00 35.40	E
MOTA	5791 5792			E 180	74.948	65.167	18.752	1.00 34.58	E
ATOM	5793	C		E 180	70.967	63.405	18.463	1.00 40.35	E
ATOM	5794	0		E 180	70.386	63.003	17.456	1.00 40.67	E
ATOM	5795	N		E 181	70.338	63.943	19.503	1.00 42.97	E
ATOM	5796	CA	GLN	E 181	68.895	64.141	19.504	1.00 45.09	E
ATOM	5797	CB	GLN	E 181	68.466	64.877	20.776	1.00 46.73	E
ATOM	5798	CG	GLN	E 181	69.471	65.931	21.235	1.00 49.84	E
MOTA	5799	CD	$\mathtt{G} L N$	E 181	68.898	66.904	22.256	1.00 52.17	E
ATOM	5800	OE1		E 181	68.074	67.760	21.920	1.00 52.91	E
ATOM	5801	NE2		E 181	69.329	66.774	23.510	1.00 51.73	E
MOTA	5802	C	•	E 181	68.607 67.660	65.002 64.752	18.277 17.530	1.00 45.26 1.00 46.25	e e
ATOM ATOM	5803 5804	N O		E 181 E 182	69.448	66.013	18.078	1.00 44.33	E
ATOM	5805	CA		E 182	69.335	66.923	16.943	1.00 42.52	E
ATOM	5806	CB		E 182	68.819	68.291	17.401	1.00 43.41	E
ATOM	5807	OG		E 182	69.658	68.853	18.396	1.00 43.07	E
MOTA	5808	C	SER	E 182	70.725	67.068	16.337	1.00 41.70	E
ATOM	5809	0	SER	E 182	71.726	66.955	17.040	1.00 39.94	E
ATOM	5810	N	PRO	E 183	70.805	67.330	15.023	1.00 41.57	E
MOTA	5811	CD		E 183	69.680	67.554	14.098	1.00 41.72	E
MOTA	5812	CA		E 183	72.087	67.485	14.326	1.00 40.68	E
ATOM	5813	CB	PRO		71.669	67.638	12.865	1.00 40.95	E
MOTA	5814	CG	PRO		70.344 72.988	68.309 68.628	12.965 14.790	1.00 42.76 1.00 38.81	E E
ATOM ATOM	5815 5816	С О		E 183 E 183	72.520	69.709	15.142	1.00 38.61	E
ATOM	5817	И	ILE		74.291	68.370	14.785	1.00 37.31	E
ATOM	5818	CA		E 184	75.270	69.368	15.177	1.00 34.30	E
ATOM	5819	CB		E 184	76.570	68.728	15.699	1.00 33.43	E
MOTA	5820	CG2	ILE	E 184	77.671	69.779	15.766	1.00 32.87	E
ATOM	5821	CG1	ILE	E 184	76.337	68.112	17.076	1.00 33.53	E
ATOM	5822	CD1	ILE	E 184	77.530	67.339	17.604	1.00 33.29	E
MOTA	5823	C		E 184	75.625	70.216	13.974	1.00 33.68	E
ATOM	5824	0		E 184	75.851	69.704	12.882	1.00 33.87	E
ATOM	5825	N		E 185	75.676	71.521	14.181	1.00 34.19	E
ATOM	5826	CA		E 185	76.018	72.431	13.111	1.00 33.39 1.00 33.77	E E
ATOM	5827	CB		E 185	74.792 74.211	73.230 73.918	12.637 13.751	1.00 33.77	E
ATOM ATOM	5828 5829	OG1 CG2			73.758	72.297	12.016	1.00 33.35	E
ATOM	5830	C	THR		77.081	73.396	13.590	1.00 33.01	E
ATOM	5831	0		E 185	76.990	73.966	14.679	1,00 33.25	E
ATOM	5832	N			78.106	73.552	12.770	1.00 32.85	E
ATOM	5833	CA		E 186	79.197	74.453	13.067	1.00 32.84	E
ATOM	5834	CB	VAL	E 186	80.503	73.684	13.300	1.00 31.58	E
MOTA	5835	CG1		E 186	81.629	74.651	13.611	1.00 30.07	E
ATOM	5836	CG2		E 186	80.316	72.697	14.441	1.00 30.84	E
MOTA	5837	C		E 186	79.329	75.317	11.836	1.00 34.14	E
MOTA	5838	0	VAL	E 186	79.403	74.812	10.719	1.00 33.50	E E
MOTA	5839	N		E 187	79.329	76.626	12.029	1.00 38.05 1.00 40.60	E
ATOM ATOM	5840 5941	CA		E 187	79.453 78.358	77.522 78.592	10.898 10.934	1.00 43.36	E
MOTA	5841	CB	GLU	то,	,0.358			T.00 -50.00	ننډ
						4 6	7 0		

T) TITONS	E049	aa	CITIT	הנ	107	70 40	م	70 521	12.121	1 00	47.46	177
ATOM	5842	CG		E	187	78.42		79.531				E
ATOM	5843	CD		E	187	77.65		80.822	11.886	1.00	51.49	E
ATOM	5844	OE1	GLU	E	187	76.45	2	80.752	11.551	1.00	52.89	E
MOTA	5845	OE2	${ t GLU}$	E	187	78.26	2	81.908	12.039	1.00	53.48	E
ATOM	5846	C	GLU	E	187	80.81	9	78.182	10.877	1.00	40.49	E
ATOM	5847	0	GLU	E	187	81.49	6	78.285	11.901	1.00	40.26	E
ATOM	5848	N	TRP	Ε	188	81.22		78.610	9.688	1.00	41.52	E
			TRP	E	188	82.49		79.284	9.488	1.00	43.59	E
ATOM	5849	CA										
ATOM	5850	CB	TRP	E	188	83.49		78.337	8.834	1.00	41.24	E
MOTA	5851	CG	TRP	\mathbf{E}	188	84.85	2	78.942	8.675	1.00	41.34	E
ATOM	5852	CD2	TRP	E	188	85.32	7	79.672	7.543	1.00	40.23	E
ATOM	5853	CE2	TRP	E	188	86.64	2	80.090	7.838	1.00	41.87	${f E}$
MOTA	5854	CE3	TRP	E	188	84.76	8	80.015	6.305	1.00	40.90	E
ATOM	5855	CD1	TRP	E	188	85.86		78.945	9.588		41.88	E
ATOM	5856	NE1	TRP	E	188	86.94		79.632	9.093		41.99	E
MOTA	5857	CZ2	TRP	E	188	87.41	1.	80.835	6.938	1.00	42.93	E
MOTA	5858	CZ3	TRP	E	188	85.53	1	80.757	5.408	1.00	42.58	E
ATOM	5859	CH2	TRP	E	188	86.83	9	81.159	5.731	1.00	43.65	E
MOTA	5860	C	TRP	E	188	82.19	8	80.467	8.566	1.00	46.04	E
ATOM	5861	0	TRP	E	188	81.33		80.374	7.688	1.00	45.30	E
									8.765	1.00	50.26	E
ATOM	5862	N	ARG	E	189	82.89		81.579				
MOTA	5863	CA		E	189	82.67		82.761	7.936	1.00	54.31	E
ATOM	5864	CB	ARG	E	189	81.98	0	83.855	8.755	1.00	56.19	E
ATOM	5865	CG	ARG	E	189	82.82	0	84.460	9.880	1.00	59.58	E
ATOM	5866	CD	ARG	E	189	83.03	0	83.499	11.045	1.00	63.51	E
ATOM	5867	NE	ARG		189	83.58	O	84.180	12.218	100	66.73	E
						84.77		84.771	12.255	1.00	68.44	E
ATOM	5868	CZ	ARG		189							
MOTA	5869	NH1	ARG		189	85.55		84.766	11.183	1.00		E
MOTA	5870	NH2	ARG	E	189	85.17	8	85.378	13.363	1.00	70.13	E
ATOM	5871	C	ARG	E	189	83.95	0	83.322	7.313	1.00	55.74	E
ATOM	5872	0	ARG	E	189	85.04	3	83.182	7.866	1.00	56.16	E
ATOM	5873	N	ALA	F.	190	83.79	6	83.962	6.156	1.00	58.53	E
ATOM	5874	CA	ALA		190	84.92		84.557	5.435	1.00		E
												E
ATOM	5875	CB	ALA		190	84.55		84.734	3.964		59.97	
MOTA	5876	C	ALA	E	190	85.33		85.905	6.036		61.01	E
ATOM	5877	0	ALA	\mathbf{E}	190	84.65	4	86.378	6.971	1.00	62.25	E
ATOM	5878	OXT	ALA	\mathbf{E}	190	86.33	8	86.479	5.558	1.00	61.85	臣
MOTA	5879	С	\mathtt{LEU}	\mathbf{F}	1	78.71	.8	38.094	33.366	1.00	32.03	F
ATOM	5880	0	LEU	F	1	79.81	.8	38.571	33.658	1.00	30.77	Ŧ
ATOM	5881	N	LEU		_ 1	76.21		38.100	33.307			F
								38.678	33.953		32.59	F
MOTA	5882	CA	LEU		1.	77.43						F
ATOM	5883	N	GLN		2	78.57		37.069	32.531		30.39	
ATOM	5884	CA	GLN	F	2	79.74	4	36.436	31.936		28.84	F
MOTA	5885	C	GLN	\mathbf{F}	2	79.60	9	36.081	30.462	1.00	27.93	F
ATOM	5886	0	GLN	F	2	78.74	1	35.308	30.067	1.00	27.68	F
ATOM	5887	N	PRO	F	3	80.46	3	36.663	29.619	1.00	28.02	F
MOTA	5888	CD		F	3	81.46		37.720	29.856	1.00	28.68	F
		CA		F	3	80.37		36.332	28.198	1.00		F
ATOM	5889											F
MOTA	5890	CB	PRO		3	81.36		37.298	27.552	1.00		
MOTA	5891	CG	PRO		3	82.35		37.575	28.660	1.00		F
MOTA	5892	C	PRO	F	3	80.77	4	34.872	28.030	1.00	27.24	F
MOTA	5893	0	PRO	F	3	81.69	8	34.406	28.698	1.00	27.18	F
ATOM	5894	N	PHE	F	4	80.08	32	34.144	27.159	1.00	25.22	F
ATOM	5895	CA	PHE	F	4	80.40	9	32.738	26.943	1.00	24.75	F
ATOM	5896	CB	PHE	F	4	79.13	_	31.905	26.849		25.85	F
			PHE	F		79.27		30.539	27.446		31.58	F
ATOM	5897	CG			4							
ATOM	5898	CD1	PHE	£,	4	79.43		30.384	28.823		33.24	F -
MOTA	5899	CD2	PHE	F	4	79.24	1	29.404	26.639	1.00	32.15	F
ATOM	5900	CE1	PHE	F	4	79.56	1	29.116	29.386	1.00	33,28	F
ATOM	5901	CE2	PHE	F	4	79.36	54	28.136	27.187	1.00	33.29	F
MOTA	5902	CZ	PHE	F	4	79.52	24	27.989	28.565	1.00	34.18	F
ATOM	5903	C	PHE	F	4	81.22		32.588	25.664	1 00	22.43	F
									24.586		24.59	- F
MOTA	5904	0	PHE	ਜ ਯ	4	80.75		32.919				
ATOM	5905	N	PRO	F	5	82.46		32.065	25.771		22.79	F
MOTA	5906	CD	PRO	F		83.19	31	31.820	27.029		21.18	F
MOTA	5907	CA	PRO	F	5	83.34	19	31.882	24.618	1.00	21.18	F
ATOM	5908	СВ	PRO	F	5	84.71	L 5	32.140	25.218	1.00	20.19	F
ATOM	5909	CG	PRO			84.58	37	31.450	26.544	1.00	20.99	F
ATOM	5910	C	PRO			83.29		30.524	23.949	1.00	20.28	F
			PRO			82.79		29.559	24.521		19.48	F
ATOM	5911	0									21.24	
ATOM	5912	N	GLN			83.81		30.456	22.730			F
MOTA	5913	CA			_	83.84		29.200	21.983		19.98	F
MOTA	5914	CB	GLN			83.66	55	29.450	20.484		18.71	F
ATOM	5915	CG	GLN	F	6	82.31	L2	30.010	20.048	1.00	18.35	F

ATOM	5916	CD	GLN	F	6	82.255	30.247	18.537	1.00 22.29	F
ATOM	5917	OE1	GLN	F	6	82,612	29.368	17.740	1.00 21.53	F
ATOM	5918	NE2	GLN	F	6	81.802	31.429	18.138	1.00 20.02	F
ATOM	5919	C	GLN	F	6	85.213	28.548	22.213	1.00 20.47	F
ATOM	5920	0	GLN	F	6	86.243	29.204	22.099	1.00 18.48	F
									1.00 21.16	F
ATOM	5921	N	PRO	F	7	85.229	27.256	22.575		
MOTA	5922	CD	PRO	\mathbf{F}	7	84.071	26.494	23.084	1.00 20.59	F
ATOM	5923	CA	PRO	F	7	86.471	26.520	22.813	1.00 21.61	F
									1.00 23.40	F
ATOM	5924	CB	PRO	F	7	86.037	25.444	23.797		
MOTA	5925	CG	PRO	F	7	84.649	25.123	23.311	1.00 19.67	F
ATOM	5926	C	PRO	F	7	86.996	25.897	21.521	1.00 23.00	F
				F	7	86.219	25.601	20.610	1.00 23.19	F
ATOM	5927	0	PRO							
MOTA	5928	N	GLU	F	8	88.312	25.714	21.438	1.00 21.78	F
ATOM	5929	CA	GLU	F	8	88.904	25.068	20.279	1.00 23.12	F
ATOM	5930	СВ	GLU	F	8	90.297	25.632	19.968	1.00 24.50	F
										F
MOTA	5931	CG	GLU	F	8	91.086	24.834	18.915	1.00 26.16	
ATOM	5932	CD	\mathtt{GLU}	F	8	90.360	24.697	17.576	1.00 31.57	\mathbf{F}
ATOM	5933	OE1	GLU	F	8	89.250	24.114	17.540	1.00 33.65	F
		OE2	GLU		8	90.903	25.171	16.555	1.00 30.66	F
MOTA	5934									
ATOM	5935	C	GLU	F	8	89.005	23.608	20.680	1.00 22.95	F
ATOM	5936	0	GLU	F	8	89.289	23.292	21.833	1.00 23.25	F
ATOM	5937	N	LEU	F	9	88.756	22.712	19.741	1.00 24.74	\mathbf{F}
									1.00 27.30	F
ATOM	5938	CA	LEU	F	9	88.815	21.292	20.047		
MOTA	5939	CB	LEU	F	9	87.729	20.549	19.272	1.00 25.73	\mathbf{F}
ATOM	5940	CG	LEU	F	9	86.302	21.051	19.494	1.00 29.20	F
					_	85.338	20.235	18.645	1.00 28.18	F
ATOM	5941		LEU		9			· · · · -		
ATOM	5942	CD2	LEU	F	9	85.938	20.943	20.967	1.00 29.61	F
ATOM	5943	C	LEU	F	9	90.178	20.707	19.712	1.00 28.17	F
ATOM	5944	0	LEU	F	9	90.715	20.940	18.631	1.00 26.94	F
ATOM	5945	N	PRO	F	10	90.765	19.947	20.647	1.00 30.38	F
ATOM	5946	CD	PRO	F	10	90.365	19.707	22.044	1.00 30.47	F
ATOM	594 7	CA	PRO	F	10	92.076	19.355	20.370	1.00 34.24	F
										F
ATOM	5948	CB	PRO	F'	10	92.556	18.915	21.752	1.00 32.97	
ATOM	5949	CG	PRO	F	10	91.282	18.561	22.448	1.00 31.98	F
MOTA	5950	C	PRO	F	10	91.985	18.188	19.393	1.00 35.94	F
							17.461	19.376	1.00 38.70	F
ATOM	5951	0	PRO	F	10	90.993				
MOTA	5952	N	TYR	\mathbf{F}^{ι}	11	93.016	18.031	18.570	1.00 37.40	F
MOTA	5953	CA	TYR	F	11	93.075	16.936	17.609	1.00 38.84	F
ATOM	5954	CB	TYR		11	92,126	17.176	16.434	1.00 38.73	F
ATOM	5955	CG	TYR	F	11	92.017	15.969	15.539	1.00 39.56	F
MOTA	5956	CD1	TYR	F	11	91.294	14.848	15.942	1.00 39.88	${f F}$
ATOM	5957	CE1	TYR	ਜਾ	11	91,254	13.697	15.164	1.00 39.49	F
										F
ATOM	5958	CD2	TYR	F	11	92.698	15.913	14.327		
MOTA	5959	CE2	TYR	F	11	92.668	14.765	13.537	1.00 40.44	F
ATOM	5960	CZ	TYR	F	11	91.945	13.659	13.964	1.00 40.29	F
	5961	OH	TYR	F	11	91.921	12.514	13.200	1.00 40.03	F
ATOM										
MOTA	5962	C	TYR	F	11	94.498	16.781	17.077	1.00 40.23	F
ATOM	5963	0	TYR	F	11	95.102	15.708	17.300	1.00 41.88	F
ATOM	5964	OXT	TYR	ਜ	11	94.988	17.742	16.443	1.00 40.58	F
								17.272	1.00 17.47	Н
MOTA	5965	0	HOH		1.	37.560	11.197			
ATOM	5966	0	HOH	H	2	81.295	26.543	20.573	1.00 15.95	H
ATOM	5967	0	HOH	H	3	43.884	23.627	16.726	1.00 14.83	H
ATOM	5968	0	нон	H	4	89.230	61.015	16.512	1.00 19.10	н
										H
ATOM	5969	0	HOH		5	92.090	40.877	18.768	1.00 15.59	
ATOM	5970	0	HOH	H	6	57.686	14.054	4.407	1.00 20.02	H
ATOM	5971	0	HOH	H	7	87.607	31.423	22.217	1.00 11.29	H
	5972	0	HOH		8	31.815	41.479	5.673	1.00 23.91	Н
ATOM										
ATOM	5973	O	HOH	H	9	46.112	3.594	18.714	1.00 20.15	H
ATOM	5974	0	HOH	H	10	86.724	67.786	15.551	1.00 22.39	, H
MOTA	5975	0	HOH	Ħ	11	42.599	14.833	17.213	1.00 16.12	H
									1.00 15.03	H
ATOM	5976	0	HOH		12	93.679	37.081	11.737		
ATOM	5977	0	HOH	H	13	50.288	0.581	25.262	1.00 13.69	H
MOTA	5978	0	HOH	H	1.4	96.256	37.853	25.291	1.00 12.90	H
		Ö	нон		15	90.711	30,936	37.307	1.00 31.88	H
ATOM	5979									
MOTA	5980	0	HOH	H	16	80.045	39.846	25.144	1.00 33.11	H
MOTA	5981	0	HOH	H	17	80.708	45.662	11.514	1.00 41.56	H
	5982	0	нон		18	42.215	0.119	11.193	1.00 15.83	H
ATOM		_								
ATOM	5983	0	HOH		19	95.828	50.485	5.930	1.00 27.67	H
MOTA	5984	0	HOH	H	20	48.809	37.278	14.928	1.00 36.10	H
ATOM	5985	0	HOH	H	21	47,553	-0.403	11.823	1.00 14.62	H
					22	94.554	76.132	19.122	1.00 83.80	н
ATOM	5986	0	HOH							
MOTA	5987	0	HOH	H	23	83.295	48.460	17.328	1.00 17.64	H
ATOM	5988	0	HOH	H	24	88.976	42.102	7.818	1.00 26.11	H
		0	HOH		25	99.041	56.322	24.823	1.00 24.86	H
MOTA	5989	<u> </u>		~ -		ンン・ 0 マル	~~.~~			•

ATOM	5990	0	нон н	26	47.640	0.006	20.312	1.00 18.95	н
ATOM	5991	0	HOH H	27	46.987	29.359	11.916	1.00 21.84	Ħ
MOTA	5992	0	HOH H	28	88.283	37.229	11.279	1.00 21.34	H
		_				-9.043		1 00 22 47	
ATOM	5993	0	HOH H	29	49.878	-9.043	36.424	1.00 32.47	H
ATOM	5994	0	нон н	30	82.777	39.366	24.935	1.00 24.79	H
ATOM	5995	0	нон н	31	72.919	25.704	15.123	1.00 18.09	Н
	3773	U							
ATOM	5996	0	HOH H	32	86.830	25.153	13.558	1.00 24.14	H
		0	UOU U	33	42 152		13.774	1,00 19,96	H
ATOM	5997	0	HOH H	23	43.152	5.651	13.//4	T'00 T3'30	
ATOM	5998	0	нон н	34	100.654	27.732	5.367	1.00 34.73	H
		^	MOH H	35	40 EEO	32.122	26.894	1.00 20.17	H
MOTA	5999	0	HOH H		48.550				
ATOM	6000	0	HOH H	36	78.728	36.578	6.822	1.00 32.92	H
ATOM	6001	0	нон н	37	89.361	11.980	24.953	1.00 51.75	н
MOTA	6002	0	HOH H	38	90.411	24.657	31.926	1.00 28.29	H
MOTA	6003	0	нон н	39	80.690	24.233	8.462	1.00 22.43	H
ATOM	6004	0	HOH H	40	83.769	65.973	-5.489	1.00 21.06	H
MOTA	6005	0	HOH H	41	87.710	34.692	7.008	1.00 22.47	H
ATOM	6006	0	HOH H	42	38.997	4.521	15.299	1.00 25.36	H
MOTA	6007	0	HOH H	43	94.223	46.644	24.674	1.00 32.67	H
								1.00 29.03	H
MOTA	6008	0	нон н	44	35.150	15.757	26.294	1.00 29.03	
ATOM	6009	0	HOH H	45	85.059	24.652	18.280	1.00 25.63	H
ATOM	6010	0	нон н	46	67.739	6.320	18.991	1.00 43.67	н
MOTA	6011	0	HOH H	47	92.376	63.977	12.866	1.00 32.46	H
ATOM	6012	0	нон н	48	91.526	49.479	22.504	1.00 29.70	H
ATOM	6013	0	HOH H	49	56.333	-2.088	24.733	1.00 28.53	H
ATOM	6014	0	нон н	50	100.482	53.937	3.942	1.00 52.26	H
		_							
ATOM	6015	0	HOH H	51	48.244	18.753	22.918	1.00 44.88	H
ATOM	6016	0	HOH H	52	32.577	-0.558	6.769	1.00 33.70	H
MOTA	6017	0	HOH H	53	47.162	26.527	12.972	1.00 29.72	H
MOTA	6018	0	HOH H	54	98.621	66.834	5.100	1.00 52.20	H
						52.134	17.293	1.00 21.13	H
ATOM	6019	0	HOH H	55	88.106				
ATOM	6020	Q	HOH H	56	59.655	31.307	17.069	1.00 25.89	H
ATOM	6021	0	нон н	57	73.562	24.323	12.997	1.00 23.51	H
MOTA	6022	0	HOH H	58	43.748	32.725	20.165	1.00 52.72	H
ATOM	6023	0	нон н	59	26.392	-7.072	11.400	1.00 26.20	H
MOTA	6024	0	HOH H	60	83.955	73.751	16.805	1.00 18.19	H
ATOM	6025	0	HOH H	61	46.229	-19.766	10.675	1.00 28.79	H
						20 720	16.630	1.00 28.35	H
ATOM	6026	0	HOH H	62	52.436	38.720			
MOTA	6027	0	HOH H	63	60.555	9.392	19.914	1.00 28.43	H
		^	нон н	64	62.105	2.197	11.948	1.00 33.33	Н
ATOM	6028	0							
ATOM	6029	0	HOH H	65	40.514	-12.059	13.631	1.00 21.32	H
ATOM	6030	0	нон н	66	65.876	23.972	14.155	1.00 21.11	Н
		_							
ATOM	6031	0	HOH H	67	84.702	18.013	5.666	1.00 19.12	H
ATOM	6032	0	HOH H	68	64.715	11.655	15.936	1.00 28.72	H
		_							
MOTA	6033	0	HOH H	69	85.418	74.949	14.820	1.00 27.90	H
MOTA	6034	0	HOH H	70	77.974	25.419	23.038	1.00 42.15	H
		^	нон н	71	65.805	8.484	20.741	1.00 44.01	H
ATOM	6035	0	non n						
MOTA	6036	0	HOH H	72	51.276	26.045	10.800	1.00 28.36	H
ATOM	6037	0	нон н	73	65.226	22.195	25.831	1.00 36.11	H
ATOM	6038	0	HOH H	74	101.567	46.068	1.107	1.00 53.81	H
ATOM	6039	0	HOH H	75	32.615	31.234	1.517	1.00 21.03	H
						-0.001	13.802	1.00 23.44	Н
ATOM	6040	0	нон н	76	42.100				
ATOM	6041	0	HOH H	77	35.124	40.614	14.668	1.00 27.61	H
ATOM	6042	0	нон н	78	92.548	46.813	7.595	1.00 31.64	H
ATOM	6043	0	HOH H	79	34.670	13.941	14.778	1.00 22.87	H
ATOM	6044	0	нон н	80	98.527	27.671	28.270	1.00 42.07	H
								1 00 27 52	Н
ATOM	6045	0	HOH H	81	30.588	36.032	16.540	1.00 37.52	
ATOM	6046	0	HOH H	82	89.345	42.957	13.940	1.00 22.73	H
	6047	\circ	нон н	83	92.891	18.085	10.698	1.00 32.35	Н
ATOM		0							
ATOM	6048	0	HOH H	84	90.050	48.556	16.519	1.00 27.30	H
ATOM	6049	0	нон н	85	110.812	49.549	15.813	1.00 27.68	H
MOTA	6050	0	HOH H	86	75.872	21.668	2.499	1.00 39.37	H
ATOM	6051	0	нон н	87	52.567	14.010	7.270	1.00 34.20	H
MOTA	6052	0	HOH H	88	69.016	32.569	12.651	1.00 36.96	H
ATOM	6053	0	нон н	89	96.637	25.945	31.742	1.00 37.26	H
									H
MOTA	6054	0	HOH H	90		-12.998	8.560	1.00 22.82	
MOTA	6055	0	HOH H	91	113.021	48.469	17.945	1.00 47.59	H
		_		92	34.266		23.930	1.00 31.02	H
ATOM	6056	0	HOH H						
MOTA	6057	0	HOH H	93	51.464	31.946	19.300	1.00 15.75	H
MOTA	6058	0	нон н	94	80.054	50.912	15.041	1.00 25.94	H
ATOM	6059	0	HOH H	95	40.413	-13.432	16.393	1.00 39.73	H
ATOM	6060	0	нон н	96	57.701	4.191	7.708	1.00 25.27	H
		_							
MOTA	6061	0	HOH H	97	80.838	52.853	26.436	1.00 27.67	H
ATOM	6062	0	нон н	98	58.205	13.023	20.294	1.00 27.57	H
							15.601	1.00 27.32	H
ATOM	6063	0	HOH H	99	41.832	30.437	TO.00T	1.00 A1.34	n

ATOM	6064	0	HOH H 100	72.807	29.880	11.618	1.00 28.05	H
ATOM	6065	0	HOH H 101	48.499	5.079	4.053		
		_						H
MOTA	6066	0	HOH H 102	100.679	66.408	9.019	1.00 36.21	H
ATOM	6067	0	HOH H 103	45.023	41.442	11.747	1.00 42.72	Ħ
ATOM	6068	0	HOH H 104	83.296	63.483	-2.738	1.00 27.46	H
ATOM	6069	0	HOH H 105	85.067	29.522	34.732	1.00 35.62	H
ATOM	6070	0	HOH H 106	72.272	53.390	15.314	1.00 38.75	H
ATOM	6071	0	HOH H 107	80.600	27.688	5.225	1.00 26.04	H
ATOM	6072	0	HOH H 108	71.251	18.567	16.503	1.00 29.08	H
ATOM	6073	0	нон н 109	88.274	65.356	19.510	1.00 26.70	H
		_						
MOTA	6074	0	HOH H 110	43.031	4.836	7.813	1.00 38.59	H
ATOM	6075	0	HOH H 111	101.304	35.384	4.755	1.00 43.53	H
MOTA	6076	0	HOH H 112	44.554	10.725	19.619	1.00 21.38	H
ATOM	6077	0	HOH H 113	115.506	34.478	5.615	1.00 46.62	H
ATOM	6078	0	HOH H 114	36.124	-25.634	9.802	1.00 42.69	H
MOTA	6079	0	нон н 115	34.494	-33.304	20.170	1.00 61.12	H
MOTA	6080	0	HOH H 116	38.663	26.161	-2.715	1.00 31.39	H
ATOM	6081	0	HOH H 117	105.197	41.384	18.739	1.00 38.53	H
MOTA	6082	0	HOH H 118	38.437	-12.372	18.422	1.00 32.47	H
ATOM	6083	0	HOH H 119	45.430	15.732	9.556	1.00 32.39	H
ATOM	6084	0	нон н 120	70.475	9.817	-1.029	1.00 53.38	H
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MOTA	6085	0	HOH H 121	87.895	64.540	22.445	1.00 47.01	H
ATOM	6086	0	HOH H 122	39.337	36.650	16.644	1.00 25.21	H
MOTA	6087	0	HOH H 123	104.091	50.783	20.204	1.00 31.31	H
MOTA	6088	0	HOH H 124	72.528	13.825	20.909	1.00 62.81	H
ATOM	6089	0	HOH H 125	55.353	-5.411	5.747	1.00 25.46	H
MOTA	6090	0	HOH H 126	97.848	63.704	25.177	1.00 27.84	H
ATOM	6091	0	HOH H 127	89.799	75.117	14.074	1.00 49.56	H
ATOM	6092	0	HOH H 128	96.226	35.565	0.211	1.00 40.25	H
ATOM	6093	0	HOH H 129	25.125	-15.445	19.161	1.00 37,04	н
MOTA	6094	0	HOH H 130	90.627	52.974	9.649	1.00 22.70	H
ATOM	6095	0	HOH H 131	114.398	29.773	11.425	1.00 42.36	H
MOTA	6096	0	нон н 132	69.810	89.608	-0.164	1.00 53.48	H
ATOM	6097	0	HOH H 133	99.069	30.421	4.728	1.00 31.21	H
MOTA	6098	0	HOH H 134	37.335	49.129	5.746	1.00 43.90	H
MOTA	6099	0	HOH H 135	77.753	73.821	17.600	1.00 50.43	H
ATOM	6100		HOH H 136	44.853	33.208	11.090	1.00 21.26	н
		0						
MOTA	6101	0	HOH H 137	88.697	80.608	-4.574	1.00 49.42	H
ATOM	6102	0	HOH H 138	62.018	-6.136	9.010	1.00 30.19	H
ATOM	6103	^	HOH H 139	35.964	-5.810	5.494	1.00 45.47	H
		0						
MOTA	6104	0	HOH H 140	73.968	65.480	8.013	1.00 43.93	H
MOTA	6105	0	HOH H 141	78.361	66.868	24.455	1.00 57.76	H
	6106	0	HOH H 142	53.527	3.199	22.332	1.00 32.95	Ħ
ATOM								
MOTA	6107	0	HOH H 143	56.018	-6.530	25.205	1.00 42.75	H
ATOM	6108	0	HOH H 144	82.930	52.617	28.345	1.00 32.35	H
ATOM	6109	0	HOH H 145		-21.313	24.210	1.00 48.87	Н
MOTA	6110	0	HOH H 146	86.079	41.197	35.698	1.00 36.97	H
ATOM	6111	0	HOH H 147	35.017	8.399	11.516	1.00 32.21	H
ATOM	6112	0	нон н 148	25.864	-19.905	17.166	1.00 41.53	Ħ
MOTA	6113	0	HOH H 149	55.504	20.659	6.959	1.00 36.63	H
ATOM	6114	0	HOH H 150	106.046	47.260	19.571	1.00 30.60	H
ATOM	6115	0	HOH H 151	108.769	26.147	5.447	1.00 48.82	H
MOTA	6116	0	HOH H 152	38.689	17.576	4.331	1.00 39.07	H
ATOM	6117	0	HOH H 153	97.787	62.580	8.740	1.00 29.61	H
ATOM	6118	0	HOH H 154	59.501	-12.817	20.769	1.00 50.36	H
ATOM	6119		HOH H 155	47.887	40.072	-4.641	1.00 51.05	Н
		0						
MOTA	6120	0	HOH H 156	60.057	16.564	27.477	1.00 40.66	H
ATOM	6121	0	HOH H 157	67.048	27.841	20.873	1.00 39,66	H
ATOM	6122	0	нон н 158	37.028	32.932	18.669	1.00 37.23	Н
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MOTA	6123	0	HOH H 159	121.780	18.693	-3.076	1.00 46.64	H
ATOM	6124	0	HOH H 160	39.196	18.091	27.271	1.00 29.99	H
ATOM	6125	O	HOH H 161	113.285	44.237	19.561	1.00 39.04	H
ATOM	6126	0	HOH H 162	43.379	27.754	19.370	1.00 27.58	H
MOTA	6127	0	HOH H 163	91.636	66.903	11.885	1.00 54.73	H
ATOM	6128	0	HOH H 164	113.381	46.844	20.020	1.00 54.22	H
MOTA	6129	0	нон н 165	79.238	62.082	24.112	1.00 36.07	H
ATOM	6130	0	HOH H 166	27.985	32.355	18.424	1.00 36.25	H
ATOM	6131	0	нон н 167	34.709	-10.661	20.615	1.00 9.89	H
								H
MOTA	6132	0	нон н 168	93.577	37.339	20.182	1.00 14.03	
ATOM	6133	0	HOH H 169	97.912	51.662	7.309	1.00 24.22	H
ATOM	6134	0	нон н 170	69.616	4.375	18.521	1.00 38.01	н
ATOM	6135		HOH H 171	80.870	25.194	6.002	1.00 21.84	H
		0						
ATOM	6136	O	HOH H 172	50.564	12.887	5.906	1.00 32.25	H
ATOM	6137	0	нон н 173	88.207	37.288	13.919	1.00 19.68	H

ATOM	6138	0	HOH H 174	93.800	47.651	27.174	1.00 41.65	н
ATOM	6139	0	HOH H 175	52.842	0.304	25.210	1.00 28.07	H
ATOM	6140	0	HOH H 176	66.457	4.742	14.051	1.00 28.64	H
ATOM	6141	0	HOH H 177	36.948	12.416	15.109	1.00 28.66	Н
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ATOM	6142	0	HOH H 178	103.292	41.793	7.607	1.00 28.51	H
ATOM	6143	0	HOH H 179	86.476	36.035	9.339	1.00 27.43	H
MOTA	6144	0	HOH H 180	82.262	41.159	26.845	1.00 24.13	H
ATOM	6145	0	HOH H 181	32.348	15.030	26.400	1.00 30.06	H
ATOM	6146	0	HOH H 182	69.916	30.709	14.482	1.00 42.81	Ħ
MOTA	6147	0	HOH H 183	48.060	10.142	26.751	1.00 49.12	H
ATOM	6148	0	HOH H 184	45.863	-9.131	37.252	1.00 43.70	H
MOTA	6149	0	HOH H 185	32.095	-3.806	34.251	1.00 41.46	H
MOTA	6150	0	HOH H 186	108.258	31.975	8.914	1.00 33.62	H
ATOM	6151	O	HOH H 187	99.465	64.293	8.210	1.00 54.43	H
MOTA	6152	0	HOH H 188	74.677	30.785	27.841	1.00 28.20	H
MOTA	6153	0	HOH H 189	44.953	0.968	35.892	1.00 32.25	H
ATOM	6154	0	HOH H 190	88.523	27.792	36.268	1.00 30.83	H
ATOM	6155	0	HOH H 191	37.736	8.611	11.729	1.00 38.92	H
MOTA	6156	0	HOH H 192	35.988	45.178	12.964	1.00 33.85	H
ATOM	6157	0	HOH H 193	77.222	68.027	1.401	1.00 27.02	H
ATOM	6158	0	HOH H 194	63.326	-8.764	15.926	1.00 38.46	H
ATOM	6159	0	HOH H 195	109.635	61.489	27.644	1.00 52.79	H
ATOM	6160	0	HOH H 196	101.299	67.528	11.319	1.00 38.92	H
ATOM	6161	0	HOH H 197	77.295	56.116	25.768	1.00 36.83	H
ATOM	6162	0	HOH H 198	81.538	22.288	0.320	1.00 47.08	H
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MOTA	6163	0	HOH H 199	55.989	3.900	0.756	1.00 46.35	H
ATOM	6164	0	HOH H 200	66.200	40.514	17.513	1.00 43.54	H
		-						н
ATOM	6165	0	HOH H 201	40.497	-1.046	9.238	1.00 27.84	
ATOM	6166	0	HOH H 202	57.171	27.504	8.258	1.00 52.74	H
ATOM	6167	0	нон н 203	44.592	-6.430	37.531	1.00 37.55	H
ATOM	6168	0	HOH H 204	26.892	-1.642	9.494	1.00 55.58	H
MOTA	6169	0	HOH H 205	83.350	58.389	2.759	1.00 46.24	H
ATOM	6170	0	HOH H 206	112.353	45.284	9.770	1.00 30.99	H
ATOM	6171	O	HOH H 207	86.315	23.927	16.100	1.00 41.36	H
MOTA	6172	0	HOH H 208	67.053	45.396	12.396	1.00 31.02	H
								H
ATOM	6173	0	HOH H 209	111.609				
ATOM	6174	0	HOH H 210	91.254	47.553	32.752	1.00 41.71	Ħ
MOTA	6175	0	HOH H 211	88.489	39.944	11.117	1.00 34.00	H
ATOM	6176	0	HOH H 212	104.972	69.233	16.415	1.00 37.26	H
ATOM	6177	0	HOH H 213	23.462	39.893	6.692	1.00 56.45	H
MOTA	6178	0	HOH H 214	84.114	54.447	-1.718	1.00 42.58	H
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ATOM	6179	0	HOH H 215	105.045	66.068	22.775	1.00 24.48	H
ATOM	6180	0	HOH H 216	85.378	52.388	17.025	1.00 37.91	H
MOTA	6181	0	HOH H 217	91.411	30 837	4.259	1.00 23.59	H
ATOM	6182	0	HOH H 218	99.019	37.803	25.178	1.00 37.20	H
ATOM	6183	0	HOH H 219	88.866	41.183	35.781	1.00 42.88	H
					25.931		1.00 45.53	Н
MOTA	6184	0	HOH H 220	66.946		12.530		
ATOM	6185	0	HOH H 221	83.809	61.544	-0.645	1.00 32.51	H
ATOM	6186	0	нон н 222	91.766	28.386	3.286	1.00 29.97	Н
ATOM	6187	0	HOH H 223	83.302	45.674	11.423	1.00 40.65	H
ATOM	6188	0	HOH H 224	59.198	3.628	18.904	1.00 22.61	H
ATOM	6189	0	нон н 225	34.553	-11.852	5.930	1.00 29.77	Ħ
ATOM	6190	0	HOH H 226	88.953	22.712	24.560	1.00 23.54	H
ATOM	6191	0	HOH H 227	108.379	54.102	21.160	1.00 30.79	H
ATOM	6192	Ö	нон н 228	44.957	16.820	6.827	1.00 37.14	Н
		_						
ATOM	6193	0	HOH H 229	105.872	50.217	22.393	1.00 33.77	H
ATOM	6194	0	HOH H 230	40.390	52.287	-1.729	1.00 62.00	H
								н
ATOM	6195	0	HOH H 231	103.837	27.586	24.806	1.00 50.76	
ATOM	6196	0	HOH H 232	50.931	9.397	25.207	1.00 40.65	H
ATOM	6197	0	нон н 233	64.739	2.382	27.973	1.00 46.98	H
ATOM	6198	0	нон н 234	38.363	0.460	8.402	1.00 28.58	H
ATOM	6199	0	нон н 235	73.577	50.129	18.561	1.00 36.68	H
MOTA	6200	0	нон н 236	100.912	58.519	6.876	1.00 36.99	H
			·					
ATOM	6201	0	нон н 237	100.664	26.841	26.380	1.00 36.27	H
ATOM	6202	0	нон н 238	82.528	48.080	12.484	1.00 44.97	H
		_		70.870	44.782	13.746	1.00 26.53	H
ATOM	6203	0	нон н 239					
ATOM	6204	0	HOH H 240	71.914	-9.049	17.302	1.00 59.29	H
ATOM	6205	0	HOH H 241	28.024	9.146	32.377	1.00 43.91	H
							1.00 50.20	H
MOTA	6206	0	HOH H 242	55.531	-2.470	4.880		
ATOM	6207	0	HOH H 243	63.362	16.623	21.334	1.00 30.95	H
ATOM	6208	0	HOH H 244	71.813	27.548	12.914	1.00 54.77	H
								H
MOTA	6209	0	HOH H 245	22.793	-3.930	12.731	1.00 39.10	
ATOM	6210	0	HOH H 246	73.087	44.091	34.124	1.00 47.86	H
ATOM	6211	0	нон н 247	48.717	31.774	19.850	1.00 33.46	H
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TA FITTO NA	C212	^	TIOU II 240	100 051	61.218	7.741	1.00 35.49	7.7
ATOM	6212	0	HOH H 248	100.851				H
ATOM	6213	0	HOH H 249	116.291	47.311	12.227	1.00 49.67	H
MOTA	6214	0	HOH H 250	99.469	40.748	22.418	1.00 25.82	H
MOTA	6215	0	HOH H 251	52.271	4.031	24.614	1.00 44.68	H
ATOM	6216	0	HOH H 252	106.629	40.298	32.271	1.00 59.44	H
ATOM	6217	0	нон н 253	45.587	-9.303	3.049	1.00 26.81	Н
ATOM	6218	0	HOH H 254	52.547	-9.432	27.670	1.00 45.08	Н
MOTA	6219	0	HOH H 255	75.854	21.157	27.640	1.00 42.33	H
MOTA	6220	0	нон н 256	82.119	63.444	23.430	1.00 37.84	H
MOTA	6221	0	HOH H 257	104.091	38.660	18.936	1.00 30.29	H
ATOM	6222	0	HOH H 258	79.477	56.121	8.190	1.00 39.16	H
ATOM	6223	0	нон н 259	101.351	32.257	5.631	1.00 29.94	н
MOTA	6224	o	HOH H 260	93.989	23.313	31.488	1.00 35.30	Н
MOTA	6225	0	HOH H 261	28.754	-1.723	6.977	1.00 36.90	H
ATOM	6226	0	HOH H 262	93.007	48.370	9.901	1.00 49.06	H
MOTA	6227	0	HOH H 263	82.990	88.137	9.529	1.00 39.70	H
MOTA	6228	0	HOH H 264	118.031	51.582	0.542	1.00 36.21	H
ATOM	6229	0	HOH H 265	21.682	15.046	11.602	1.00 62.29	H
MOTA	6230	0	нон н 266	34.210	24.576	5.314	1.00 18.89	H
			HOH H 267	85.829	40.095	14.911	1.00 25.26	H
ATOM	6231	0						
MOTA	6232	0	HOH H 268	102.070	38.308	21.059	1.00 41.79	H
MOTA	6233	0	нон н 269	41.071	-2.346	7.039	1.00 38.87	H
MOTA	6234	0	HOH H 270	68.717	3.686	16.083	1.00 37.79	H
ATOM	6235	0	HOH H 271	27.094	-12.649	12.753	1.00 29.26	H
ATOM	6236	0	HOH H 272	36.426	24.744	4.145	1.00 45.88	H
ATOM		o	HOH H 273	88.670	31.858	5.525	1.00 39.43	H
	6237							
ATOM	6238	0	HOH H 274	90.819	38.524	36.028	1.00 30.15	H
ATOM	6239	0	HOH H 275	90.790	49.861	10.317	1.00 39.97	H
ATOM	6240	0	HOH H 276	77.026	11.969	13.970	1.00 44.87	Ħ
ATOM	6241	0	HOH H 277	36.555	12.078	12.344	1.00 40.47	H
ATOM	6242	0	нон н 278	52.331	7.302	24.972	1.00 49.30	н
MOTA	6243	Ō	HOH H 279	92.612	33.229	3.564	1.00 40.55	H
				83.546	64.142	25.612	1.00 50.28	H
MOTA	6244	0	HOH H 280					
ATOM	6245	0	HOH H 281	28.206	-1.891	36.868	1.00 44.06	H
MOTA	6246	0	HOH H 282	93.185	20.914	30.917	1.00 44.51	H
ATOM	6247	0	HOH H 283	98.176	41.763	24.500	1.00 44.20	H
ATOM	6248	0	HOH H 284	29.174	-0.123	4.304	1.00 46.75	H
MOTA	6249	0	HOH H 285	79.206	77.643	14.919	1.00 30.21	H
ATOM	6250	0	нон н 286	90.531	26.085	37.436	1.00 36.96	H
ATOM	6251	o	HOH H 287	55.726	0.396	21.054	1.00 49.55	H
							1.00 42.91	H
MOTA	6252	0	HOH H 288	111.246	30.915	19.699		
ATOM	6253	0	HOH H 289	77.000	58.921	5.300	1.00 47.04	H
MOTA	6254	\mathbf{O}'	HOH H 290	34.339	-9.458	5.288	1.00 25.50	H
MOTA	6255	0	HOH H 291	109.784	29.168	15.534	1.00 45.96	Ħ
ATOM	6256	0	HOH H 292	93.674	48.853	29.650	1.00 48.76	H
ATOM	6257	0	нон н 293	92.299	47.066	3.801	1.00 37.41	Н
ATOM	6258	0	HOH H 294	110.965	23.141	11.799	1.00 42.97	H
						33.919	1.00 33.83	H
ATOM	6259	0	нон н 295	90.562	45.235			
MOTA	6260	0	нон н 296		-10.500	25.018	1.00 49.78	H
MOTA	6261	0	НОН Н 297	54.676	36.195	11.362	1.00 54.22	H
ATOM	6262	0	HOH H 298	107.263	59.234	5.282	1.00 56.05	H
ATOM	6263	0	HOH H 299	70.560	48.918	1.476	1.00 49.72	H
ATOM	6264	0	нон н 300	84.037	38.916	5.971	1.00 39.33	H
ATOM	6265	0	HOH H 301	86.468	41.381	11.971	1.00 45.69	Н
				24.400	11.569	23.610	1.00 36.73	H
ATOM	6266	0	HOH H 302					
ATOM	6267	0	нон н 303	73.087	79.808	7.028	1.00 46.20	H
ATOM	6268	0	HOH H 304	72.681	43.116	14.941	1.00 51.84	H
ATOM	6269	0	HOH H 305	84.844	42.198	15.611	1.00 26.23	H
ATOM	6270	0	нон н 306	54.135	19.007	24.978	1.00 27.41	H
ATOM	6271	0	нон н 307	67.044	10.459	18.465	1.00 44.92	H
ATOM	6272	ō	нон н 308	82.262	49.436	14.864	1.00 39.04	H
			HOH H 309	114.093	50.994	16.895	1.00 43.32	Н
ATOM	6273	0						
MOTA	6274	0	нон н 310	64.428	3.092	30.590	1.00 43.29	H
ATOM	6275	0	HOH H 311	81.152	70.187	18.656	1.00 34.21	H
ATOM	6276	0	HOH H 312	74.596	81.584	-2.515	1.00 55.00	H
MOTA	6277	0	нон н 313	61.161	25.774	22.464	1.00 32.98	H
ATOM	6278	0	нон н 314	53.149	-7.019	4.754	1.00 26.01	H
ATOM	6279	0	нон н 315	44.571	8.317	33.567	1.00 40.32	Н
ATOM	6280	0	нон и 316	82.293	49.769	10.587	1.00 35.22	H
				48.467	8.859	24.614	1.00 33.22	H
ATOM	6281	0	HOH H 317					
ATOM	6282	0	HOH H 318	56.588	-8.027	4.728	1.00 44.65	H
MOTA	6283	0	нон н 319	31.280		26.551	1.00 42.45	H
ATOM	6284	0	нон н 320	82.483	40.137	7.719	1.00 39.22	H
MOTA	6285	0	нон н 321	82.063	19.937	23.440	1.00 35.69	H
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6286 Q HOH H 322 106.025 63.366 22.616 1.00 31.93 \mathbf{H} MOTA HOH H 323 46.181 9.890 8.669 1.00 38.11 H MOTA 6287 0 ATOM 6288 0 HOH H 324 71.708 75.568 6.998 1.00 41.82 H 108.280 34.405 3.851 1.00 30.72 H ATOM 6289 0 HOH H 325 14.635 H MOTA 6290 0 HOH H 326 32.275 40.921 1.00 40.72 HOH H 327 37.556 15.785 5.690 1.00 42.29 H MOTA 6291 33.598 85.569 H MOTA 6292 HOH H 328 37.182 1.00 31.78 1.00 48.90 H 33.070 -11.287 23.137 ATOM 6293 HOH H 329 16.513 1.00 45.53 6294 87.593 19.683 H MOTA HOH H 330 53.631 6295 HOH H 331 116.176 17.853 1.00 39.81 H MOTA 26.940 -11.377 14.930 1.00 39.40 H ATOM 6296 HOH H 332 6297 60.033 28.679 22.456 1.00 32.84 H MOTA HOH H 333 15.182 2.562 1.00 48.72 H MOTA 6298 HOH H 334 52.472 H ATOM 6299 HOH H 335 84.377 54.588 4.646 1.00 40.99 115.759 67.454 19.970 1.00 46.15 Η ATOM 6300 HOH H 336 H MOTA 6301 HOH H 337 88.969 52.684 25.112 1.00 42.31 36.351 12.852 9.875 1.00 37.11 H MOTA 6302 HOH H 338 H 97.702 31.578 2.653 1.00 49.82 ATOM 6303 HOH H 339 -6.543 26.981 1.00 35.52 H 53.964 MOTA 6304 HOH H 340 24.475 -17.438 17.094 1.00 38.04 H HOH H 341 ATOM 6305 H MOTA 6306 HOH H 342 58.530 0.915 19.036 1.00 43.08 37.203 39.025 H 77.156 1.00 48.54 MOTA 6307 0 HOH H 343 49.978 -1.361 0.435 1.00 39.48 Η MOTA 6308 HOH H 344 53.900 37.104 13.703 1.00 47.74 H MOTA 6309 HOH H 345 0 H ATOM 6310 HOH H 346 77.886 49.625 13.575 1.00 57.13 0 0.570 1.00 50.38 H 8.721 HOH H 347 57.053 ATOM 6311 0 63.745 10.854 1.00 41.14 6312 96.803 MOTA 0 HOH H 348 89.009 70.808 11.906 1.00 45.67 H ATOM 6313 0 HOH H 349 8.221 1.00 42.47 H MOTA 6314 HOH H 350 66.363 22.353 25.044 8.541 1.00 41.16 H 52.578 6315 HOH H 351 MOTA 73.640 -3.536 1.00 50.48 H 81.789 ATOM 6316 HOH H 352 1.00 48.24 13.891 H 6317 HOH H 353 67.632 -11.181 MOTA H ~5.652 22.367 1.00 14.47 6318 HOH H 354 41.357 ATOM -5.096 30.876 1.00 23.96 G EDO G 501 37.685 6319 C1 ATOM G EDO G 501 38.224 -4.213 31.883 1.00 23.38 ATOM 6320 01 G -6.046 30.406 1.00 25.29 EDO G 501 38.742 ATOM 6321 C2 G 39.062 -6.931 31.464 1.00 26.30 6322 02 EDO G 501 ATOM G EDO G 502 89.146 26.377 27.000 1.00 41.69 MOTA 6323 Cl G EDO G 502 88.631 26.508 28.343 1.00 51.10 ATOM 6324 01 G 88.436 25.261 26.303 1.00 43.14 6325 C2 EDO G 502 ATOM 24.052 26.967 1.00 41.73 G EDO G 502 88.726 MOTA 6326 02 EDO G 503 85.093 31.920 30.633 1.00 21.00 ATOM 6327 C1 31.203 1.00 18.65 EDO G 503 85.283 30.597 ATOM 6328 Ol 32.561 31.186 1.00 19.69 6329 C2 **EDO G 503** 83.846 ATOM EDO G 503 84.148 33.101 32.454 1.00 20.94 ATOM 6330 02 G 3.907 25.885 1.00 38.01 6331 C1 EDO G 504 34.956 ATOM 2.838 25.869 1.00 36.69 G 33.976 6332 O1 EDO G 504 ATOM 3.344 25.982 1.00 39.84 G 6333 C2 EDO G 504 36.360 MOTA 2.396 24.935 1.00 33.51 36.573 6334 O2 EDO G 504 MOTA END

Example 4

Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition (IC $_{50}$) is calculated. Since the level of IC $_{50}$ may vary between separate titration experiments, the IC $_{50}$ values are compared to the IC $_{50}$ of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: IC $_{50}$ of reference peptide / IC $_{50}$ of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the β -subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of IC $_{50}$. A peptide analog with an IC $_{50}$ value of less than 100 μ M is suitable for further screenings.

Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β -subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of IC50 or K_i.

[93] Candidate peptide analogs are further tested for their ability to inhibit proliferation of T cells specific for gluten peptides. This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X 10⁴ TCC with 5 X 10⁴ fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [3H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 µM or greater are suitable for further screening.

[94] All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95] Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

1. An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

- 2. The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises one or more naturally occurring amino acids, non-naturally occurring amino acids, modified amino acids, or amino acid mimetics.
- 3. The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
- 4. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.
- 5. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.
- [96] 6. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.
 - 7. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
 - 8. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
 - 9. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PFPQX₁ELX₂Y, where X_1 and X_2 are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of X_1 and X_2 is a residue other than proline

10. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

- 11. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
- 12. A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:

administering to a patient an effective dose of an HLA-binding peptide inhibitor; wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

- 13. The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.
- 14. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.
- 15. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.
- 16. A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:

an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

- 17. The formulation according to Claim 16, further comprising an enteric coating.
- 18. Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.
- 19. A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

- a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said threedimensional representation; and
- a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 20. A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
- (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;
- (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
- (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.